

First-order definable string transformations

Emmanuel Filiot¹, Shankara Narayanan Krishna², and Ashutosh Trivedi²

¹ F.N.R.S. Research Associate
Université Libre de Bruxelles
Bruxelles, Belgium
efiliot@ulb.ac.be

² Indian Institute of Technology Bombay
Powai, Mumbai, India
krishnas,trivedi@cse.iitb.ac.in

Abstract

The connection between languages defined by computational models and logic for languages is well-studied. Monadic second-order logic and finite automata are shown to closely correspond to each-other for the languages of strings, trees, and partial-orders. Similar connections are shown for first-order logic and finite automata with certain aperiodicity restriction. Courcelle in 1994 proposed a way to use logic to define functions over structures where the output structure is defined using logical formulas interpreted over the input structure. Engelfriet and Hooeboom discovered the corresponding "automata connection" by showing that two-way generalised sequential machines capture the class of monadic-second order definable transformations. Alur and Cerny further refined the result by proposing a one-way deterministic transducer model with string variables—called the streaming string transducers—to capture the same class of transformations. In this paper we establish a transducer-logic correspondence for Courcelle’s first-order definable string transformations. We propose a new notion of transition monoid for streaming string transducers that involves structural properties of both underlying input automata and variable dependencies. By putting an aperiodicity restriction on the transition monoids, we define a class of streaming string transducers that captures exactly the class of first-order definable transformations.

1 Introduction

The class of regular languages is among one of the most well-studied concept in the theory of formal languages. Regular languages have been precisely characterized widely by differing formalisms like monadic second-order logic (MSO), finite state automata, regular expressions, and finite monoids. In particular, the connection [8] between finite state automata and monadic second-order logic is one of the celebrated results of formal language theory. Over the years, there has been substantial research to establish similar connections for the languages definable using first-order logic (FO) [12]. In particular, first-order definable languages have been shown to be precisely captured by, among others, aperiodic finite state automata. Aperiodic automata are restrictions of finite automata with certain aperiodicity restrictions on their transition matrices defined through aperiodicity of their transition monoid. Other formalisms capturing first-order definable languages include counter-free automata, star-free regular expressions, and very weak alternating automata.

Starting with the work of Courcelle [11], logic and automata connections have also been established for the theory of string transformations. The first result in this direction is by Engelfriet and Hooeboom [14], where MSO-definable transformations have been shown to be equivalent to two-way finite transducers. This result has then been extended to trees and macro-tree transducers [15]. Recently, Alur and Černý [1, 2] introduced *streaming string transducers*, a one-way finite transducer model extended with variables, and showed that they precisely capture MSO-definable transformations not only in finite string-to-string case, but also for infinite strings [6] and tree [3, 5] transformations. In this paper, we show a logic and transducer connection for first-order definable string transformations, by introducing an appropriate notion of aperiodic transition monoid for streaming string transducers.

Streaming string transducers (SSTs) manipulate a finite set of string variables to compute their output as they read the input string in one left-to-right pass. Instead of appending symbols to the output tape, SSTs concurrently update all string variables using a concatenation of output symbols and string variables in a *copyless* fashion, i.e. no variable occurs more than once in each concurrent variable update. The transformation of a string is then defined using an



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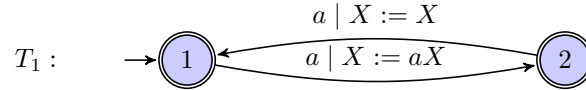
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2 First-order definable string transformations

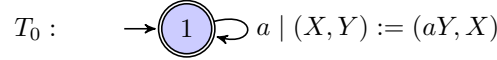
output (partial) function F that associates states with a copyless concatenation of string variables, s.t. if the state q is reached after reading the string and $F(q)=XY$, then the output string is the final valuation of X concatenated with that of Y . It has been shown that SSTs have good algorithmic properties (such as decidable type-checking, equivalence) [1, 2] and naturally generalize to various settings like trees and nested words [3, 5], infinite strings [6], and quantitative languages [4].

1.1 Aperiodic Streaming String Transducers

Let us consider transformation f_{halve} defined as $a^n \mapsto a^{\lceil \frac{n}{2} \rceil}$. Intuitively, it can be shown (see Appendix H for a proof) that f_{halve} is not FO-definable since it requires to distinguish based on the parity of the input. Consider, the following SST T_1 with 2 accepting states and 1 variable.



Readers familiar with aperiodic automata may notice that the automata corresponding to T_1 is not aperiodic, but indeed has period 2. Formally such aperiodicity is captured by the notion of automata transition monoid. The transition monoid of an automaton A is the set of Boolean transition matrices M_s , for all strings s , indexed by states of A : $M_s[p][q] = 1$ iff there exists a run from p to q on s . The set of matrices M_s is a finite monoid. It is aperiodic if there exists $m \geq 0$ such that for all $s \in \Sigma^*$, $M_{s^m} = M_{s^{m+1}}$. Aperiodic automata define exactly first-order languages [18, 12]. It seems a valid conjecture that SSTs whose transition monoid of underlying automaton is aperiodic characterize first-order definable transformations. However, unfortunately this is not a sufficient condition as shown by the following SST T_0 which also implements f_{halve} (its output is $F(1) = X$).



In this example, although the underlying automaton is aperiodic, variables contribute to certain non aperiodicity. We capture this idea by introducing the notion of variable flow. In this SST, we say that by reading letter a , variable X flows to Y (since the update of variable Y is based on variable X) while Y flows to X . We extend the notion of transition monoid for SSTs to take both state and variable flow into account. We define transition matrices M_s indexed by pairs (p, X) where p is a state and X is a variable. Since in general, for copy-full SSTs, a variable X might be copied in more than one variable, it could be that X flows into Y several times. Our notion of transition monoid also takes into account, the number of times a variable flows into another. In particular, $M_s[p, X][q, Y] = i$ means that there exists a run from p to q on s on which X flows to Y i times. Hence the transition monoid of an SST may not be finite.

1.2 Main results

In this paper we introduce a new concept of transition monoid for SST, used to define the notion of aperiodic SST. FO transformations, although weaker than MSO transducers, still enjoy a lot of expressive power: for instance they can still double, reverse, and swap strings, and are closed under FO look-ahead. We show that FO string transformations are exactly the transformations definable by SST whose transition monoid is aperiodic with matrix values ranging over $\{0, 1\}$ (called 1-bounded transition monoid). We also show that checking aperiodicity of an SST is PSPACE-COMplete. Simple restrictions on SST transition monoids nicely capture restrictions on variable updates that has been considered in other works. For instance, *bounded copy* of [6] correspond to finiteness of the transition monoid, while *restricted copy* of [3] correspond to its 1-boundedness. Finally, unlike [1], our proof is not based on the intermediate model of two-way transducers and is more direct. We give a logic-based proof that simplifies that of [5] by restricting it to string-to-string transformations.

1.3 Related work

Diekert and Gastin [12] presented a detailed survey of several automata, logical, and algebraic characterisations of first-order definable languages. As mentioned earlier the connection between MSO and transducers have been investigated in [1, 14]. Connection between two-way transducers and FO-transformations has been mentioned in [9] in an oral communication, where they left the SST connection as an open question. First-order transformations are considered in [16], but not in the sense of [11]. In particular, they are weaker, as they cannot double strings or mirror them, and are definable by one-way (variable-free) finite state transducers. Finally, [7] considers first-order definable transformations *with origin information*. The semantics is different from ours, because these transformations are not just mapping from string to strings, but they also connect output symbols with input symbols from where they originate.

The first-order definability problem for regular languages is known to be decidable. In particular, given a deterministic automaton A , deciding whether A defines a first-order language can be decided in PSPACE . Although we make an important and necessary step in answering this question in the context of regular string transformation, the decidability remains an open problem.

2 Preliminaries

2.1 Alphabets, Strings, and Languages

An alphabet Σ is a finite set of letters. A finite string over Σ is defined as a finite sequence of letters from Σ . We denote by ϵ the empty string. We write Σ^* for the set of finite strings over Σ . A (string) language over an alphabet Σ is defined as a set of finite strings.

For a string $s \in \Sigma^*$ we write $|s|$ for its length and $\text{dom}(s)$ for the set $\{1, \dots, |s|\}$. For all $i \in \text{dom}(s)$ we write $s[i]$ for the i -th letter of the string s . For any $j \in \text{dom}(s)$, the substring starting at position i and ending at position j is defined as ϵ if $j < i$ and by the sequence of letters $s[i]s[i+1] \dots s[j]$ otherwise. We write $s[i:j]$, $s(i:j)$, $s[i:j]$, and $s(i:j)$, to denote substrings of s respectively starting at i and ending at j , starting at $i+1$ and ending at $j-1$, and so on. For instance, $s[1:x]$ denotes the prefix ending at $x-1$ (it is ϵ if $x=1$), while $s(x:|s|)$ denotes the suffix starting at $x+1$.

2.2 First-order logic for strings

We represent a string $s \in \Sigma^*$ by the relational structure $\Xi_s = (\text{dom}(s), \preceq^s, (L_a^s)_{a \in \Sigma})$, called the string model of s , where

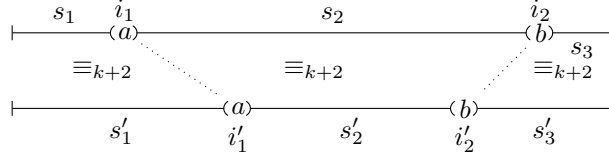
- $\text{dom}(s) = \{1, 2, \dots, |s|\}$ is the set of positions in s ,
- \preceq^s is a binary relation over the positions in s characterizing the natural order, i.e. $(x, y) \in \preceq^s$ if $x \leq y$;
- L_a^s , for all $a \in \Sigma$, are the unary predicates that hold for the positions in s labeled with the alphabet a , i.e., $L_a^s(i)$ iff $s[i] = a$, for all $i \in \text{dom}(s)$.

When it is clear from context we will drop the superscript s from the relations \preceq^s and L_a^s .

Properties of string models over the alphabet Σ can be formalized by first-order logic denoted by $\text{FO}(\Sigma)$ (or FO when Σ is clear from the context). Formulas of $\text{FO}(\Sigma)$ are built up from variables x, y, \dots ranging over positions of string models along with *atomic formulas* of the form $x=y$, $x \preceq y$, and $L_a(x)$ for all $a \in \Sigma$ where formula $x=y$ states that variables x and y points to the same position, the formula $x \preceq y$ states that position corresponding to variable x is not bigger than that of y , and the formula $L_a(x)$ states that position x has the label $a \in \Sigma$. Atomic formulas are connected with *propositional connectives* \neg , \wedge , \vee , \rightarrow , and *quantifiers* \forall and \exists that range over node variables. We say that a variable is *free* in a formula if it does not occur in the scope of some quantifier. A *sentence* is a formula with no free variables. We write $\phi(x_1, x_2, \dots, x_k)$ to denote that at most the variables x_1, \dots, x_k occur free in ϕ . For a string $s \in \Sigma^*$ and for positions $n_1, n_2, \dots, n_k \in \text{dom}(s)$ we say that s with valuation $\nu = (n_1, n_2, \dots, n_k)$ satisfies the formula $\phi(x_1, x_2, \dots, x_k)$ and we write $(s, \nu) \models \phi(x_1, x_2, \dots, x_k)$ or $s \models \phi(n_1, n_2, \dots, n_k)$ if formula ϕ with n_i as the interpretation of x_i is satisfied in the string model Ξ_s . We define the following useful FO-shorthands.

- $x \succ y \stackrel{\text{def}}{=} \neg(x \preceq y)$ and $x \prec y \stackrel{\text{def}}{=} (x \preceq y) \wedge \neg(x = y)$,
- $S(x, y) \stackrel{\text{def}}{=} (x \prec y) \wedge \forall z((z \prec y) \rightarrow (z \preceq x))$
- $\text{last}(x) \stackrel{\text{def}}{=} \neg \exists y. S(x, y)$ and $\text{first}(x) \stackrel{\text{def}}{=} \neg \exists y. S(y, x)$

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■ **Figure 1** String decomposition of Proposition 1.2

■ The sentence `is_string` characterizes valid string models and is defined as

$$\text{is_string} \stackrel{\text{def}}{=} \forall x, y, z. (\bigvee_{a \in \Sigma} L_a(x)) \wedge \bigwedge_{a \neq b \in \Sigma} (L_a(x) \rightarrow \neg L_b(x)) \wedge (S(x, y) \wedge S(x, z) \rightarrow y = z) \wedge (\text{first}(x) \wedge \text{first}(y) \rightarrow x = y).$$

It is easy to see that a structure satisfying `is_string` property uniquely characterizes a string. The language defined by an FO sentence ϕ is $L(\phi) \stackrel{\text{def}}{=} \{s \in \Sigma^* : \Xi_s \models \phi\}$. We say that a language L is FO-definable if there is an FO sentence ϕ such that $L = L(\phi)$.

► **Example 1.** Let $\Sigma = \{a, b\}$. Consider the language $L_1 \subseteq \Sigma^*$ of strings ending with b definable using the following formula $\forall x. (\text{last}(x) \rightarrow L_b(x))$. The language $L_2 = \{(ab)^n : n \geq 0\}$ is definable using the following FO formula:

$$\forall x. (\text{first}(x) \rightarrow L_a(x)) \wedge \forall x. (\text{last}(x) \rightarrow L_b(x)) \wedge \forall y. (L_a(x) \wedge S(x, y) \rightarrow L_b(y)) \wedge \forall y. (L_b(x) \wedge S(x, y) \rightarrow L_a(y))$$

First-order logic can be used, in an analogous manner, to define languages of trees and graphs by defining appropriate relational structures [19]. Monadic second-order logic extends first-order logic by permitting variables to range over sets of positions (monadic second-order variables) and quantification over such variables. We say that a language is MSO-definable if it can be characterized by an MSO sentence.

2.3 Properties of first-order logic

The *quantifier rank*, $qr(\phi)$, of an FO-formula ϕ is defined as the maximal number of nested quantifiers in ϕ , formally:

$$qr(\phi) = \begin{cases} 0 & \text{if } \phi \text{ is atomic} \\ \max \{qr(\phi_1), qr(\phi_2)\} & \text{if } \phi = \phi_1 \vee \phi_2 \text{ or } \phi_1 \wedge \phi_2 \\ qr(\phi_1) & \text{if } \phi = \neg \phi_1 \\ 1 + qr(\phi_1) & \text{if } \phi = \exists x \phi_1 \text{ or } \phi = \forall x \phi_1 \end{cases}$$

A fundamental property [18] of first-order logic states that for a given $k \in \mathbb{N}$, there are only finitely many sentences—up to logical equivalence—of quantifier rank lesser than k . Based on this property one defines the notion of first-order k -type for strings. The first-order k -type of a string s , denoted by $\langle s \rangle_k$, is the set of FO-sentences of quantifier rank at most k that are satisfied by s . Formally,

$$\langle s \rangle_k = \{\phi : \phi \text{ is an FO-sentence s.t. } qr(\phi) \leq k \wedge s \models \phi\}$$

We write $\Theta_k = \{\langle s \rangle_k \mid s \in \Sigma^*\}$ for the set of k -types. Since there are only finitely many sentences of quantifier rank lesser than k , Θ_k is finite.

We say that two strings $s, s' \in \Sigma^*$ are k -equivalent, denoted by $s \equiv_k s'$, if they have the same k -type, i.e. $\langle s \rangle_k = \langle s' \rangle_k$. In other words, s and s' are k -equivalent if they satisfy the same FO-sentences of quantifier rank at most k . It is also well-known [18] that \equiv_k is a congruence relation of finite index.

► **Proposition 1** (Properties of FO-formulas of bounded quantifier-depth [18]). In this paper we use the following fundamental properties of FO formulas.

1. For all strings $s_1, s_2, s'_1, s'_2 \in \Sigma^*$, if $s_1 \equiv_k s'_1$ and $s_2 \equiv_k s'_2$, then $s_1 s_2 \equiv_k s'_1 s'_2$.

2. For all $k \geq 0$. Let $s_1, s_2, s_3, s'_1, s'_2, s'_3 \in \Sigma^*$, and $a, b \in \Sigma$, such that $s_i \equiv_{k+2} s'_i$, $i = 1, 2, 3$. Let $i_1 = |s_1| + 1$, $i_2 = i_1 + |s_2| + 1$, $i'_1 = |s'_1| + 1$, $i'_2 = i'_1 + |s'_2| + 1$ (see Fig. 1). Let $\phi(x, y), \psi(x)$ be two FO formulas of quantifier rank at most k . We have

$$s_1as_2 \models \psi(i_1) \text{ iff } s'_1as'_2 \models \psi(i'_1) \quad \text{and} \quad s_1as_2bs_3 \models \phi(i_1, i_2) \text{ iff } s'_1as'_2bs'_3 \models \phi(i'_1, i'_2).$$
3. [18] For all $k \geq 0$ and all $m \geq 2^k$, for all strings $s, s' \in \Sigma^*$, $s^m \equiv_k s^{m+1}$, or in other words $\langle s^m \rangle_k = \langle s^{m+1} \rangle_k$.

Thanks to Proposition 1.1, one can extend the concatenation operator to types: for all $\tau_1, \tau_2 \in \Theta_k$, $\tau_1.\tau_2 = \langle s_1.s_2 \rangle_k$ where $s_1, s_2 \in \Sigma^*$ are such that $\tau_i = \langle s_i \rangle_k$, $i = 1, 2$. The operator “.” on k -types is called *type composition*.

The following proposition states that k -types can be represented by an FO sentence of quantifier-depth at most k . Moreover, the k -types of a substring of s between two positions i_1 and i_2 such that $i_1 < i_2$ can also be characterized by some FO-formula with two free variables by guarding all quantifications of any variable z in Φ_τ (τ is a k -type) by the predicate *guard*(z) = $x \preceq z \preceq y$.

► **Proposition 2** ([18]). Let Θ_k be the set of all k -types.

1. For all k -types $\tau \in \Theta_k$, there exists an FO-sentence Φ_τ of quantifier rank at most k , such that for all strings $s \in \Sigma^*$, $s \models \Phi_\tau$ iff $\langle s \rangle_k = \tau$.
2. For all k -types $\tau \in \Theta_k$, there exists an FO-formula $\Psi_\tau(x, y)$ of quantifier rank at most k such that for all strings $s \in \Sigma^*$ and all positions $i_1 < i_2$ of s , $s \models \Psi_\tau(i_1, i_2)$ iff $\langle s[i_1 : i_2] \rangle_k = \tau$.

2.4 Aperiodic finite automata

A finite automaton is a tuple $\mathcal{A} = (Q, q_0, \Sigma, \delta, F)$ where Q is a finite set of states, $q_0 \in Q$ is the initial state, Σ is an input alphabet, $\delta : Q \times \Sigma \rightarrow Q$ is a transition function, and $F \subseteq Q$ is the set of accepting states. For states $q, q' \in Q$ and letter $a \in \Sigma$ we say that (q, a, q') is a transition of the automaton \mathcal{A} if $\delta(q, a) = q'$ and we write $q \xrightarrow{a} q'$. A run of \mathcal{A} over a finite string $s = a_1a_2 \dots a_n \in \Sigma^*$ is a finite sequence of transitions $\langle (q_0, a_1, q_1), (q_1, a_2, q_2), \dots, (q_{n-1}, a_n, q_n) \rangle \in (Q \times \Sigma \times Q)^*$ starting from the initial state q_0 and we represent such runs as $q_0 \xrightarrow{a_1} q_1 \xrightarrow{a_2} q_2 \dots q_n$; also, in this case we say that there is a run of \mathcal{A} from q_0 to q_n over the string s and we write $q_0 \rightsquigarrow_{\mathcal{A}}^s q_n$ (or $q_0 \rightsquigarrow^s q_n$ if the automaton is clear from the context). A string s is accepted by a finite automaton \mathcal{A} if there exists $q_n \in F$ such that $q_0 \rightsquigarrow^s q_n$. The language defined by a finite automaton \mathcal{A} is $L(\mathcal{A}) = \{s : q_0 \rightsquigarrow^s q_n \text{ and } q_n \in F\}$.

Büchi-Elgot-Trakhtenbrot [8, 13, 20] first established the connection between mathematical logic and automata theory by showing that the deterministic finite state automata accept the same class of languages as monadic second order logic (MSO) interpreted over finite strings. This class of languages is also known as *regular languages*.

► **Theorem 2** ([8, 13, 20]). *A language $L \subseteq \Sigma^*$ is MSO-definable iff it is accepted by some finite automaton.*

To define a similar automata connection for FO-definable languages, we need to introduce the concept of aperiodic finite automata. Recall that a monoid is an algebraic structure (M, \cdot, e) with a non-empty set M , a binary operation \cdot , and an identity element $e \in M$ such that for all $x, y, z \in M$ we have that $(x \cdot (y \cdot z)) = ((x \cdot y) \cdot z)$, and $x \cdot e = e \cdot x$ for all $x \in M$. We say that a monoid (M, \cdot, e) is *finite* if the set M is finite. We say that a monoid (M, \cdot, e) is *aperiodic* [18] if there exists $n \in \mathbb{N}$ such that for all $x \in M$, $x^n = x^{n+1}$. Note that for finite monoids, it is equivalent to require that for all $x \in M$, there exists $n \in \mathbb{N}$ such that $x^n = x^{n+1}$.

► **Example 3** (Monoids). The following three monoids are useful for the development of the results presented in the paper.

- **Free Monoid.** The set of all strings over Σ forms a monoid, with string concatenation as the operation and the empty string ϵ as the identity element. This monoid is denoted as $(\Sigma^*, \cdot, \epsilon)$ and known as the free monoid.
- **k -type Monoid.** The set of k -types form a finite monoid $(\Theta_k, \cdot, \langle \epsilon \rangle_k)$ with type composition as the operation and the k -type of the empty string $\langle \epsilon \rangle_k$ as the identity element. For instance, a direct consequence of Proposition 1.(3) is aperiodicity of the monoid $(\Theta_k, \cdot, \langle \epsilon \rangle_k)$.
- **Transition Monoid** The set of transition matrices of a finite automaton $\mathcal{A} = (Q, q_0, \Sigma, \delta, F)$ forms a finite monoid with matrix multiplication as the operation and the unit matrix **1** as the identity element. This monoid is denoted

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as $\mathcal{M}_{\mathcal{A}} = (M_{\mathcal{A}}, \times, 1)$ and known as transition monoid of \mathcal{A} . Formally, the set $M_{\mathcal{A}}$ is the set of $|Q|$ -square Boolean matrices $M_{\mathcal{A}} = \{M_s : s \in \Sigma^*\}$ where for all strings $s \in \Sigma^*$, we have that $M_s[p][q] = 1$ iff $p \rightsquigarrow^s q$.

We say that a finite automaton is aperiodic if its transition monoid is aperiodic. The following is a key theorem characterizing FO-definable languages using automata.

► **Theorem 4.** [18] *A language $L \subseteq \Sigma^*$ is FO-definable iff it is accepted by some aperiodic finite automaton.*

Combining Proposition 2 and Theorem 4 it follows that for every k -type $\tau \in \Theta_k$ there is an aperiodic finite automaton A_{τ} that accepts all strings s with $\langle s \rangle_k = \tau$. Such automaton A_{τ} is defined as the tuple $A_{\tau} = (Q_{\tau} = \Theta_k, \langle \epsilon \rangle_k, \Sigma, \delta_{\tau}, F_{\tau} = \{\tau\})$, where $\delta_{\tau}(\tau', a) = \tau' \cdot \langle a \rangle_k$ for all $\tau' \in \Theta_k$ and $a \in \Sigma$. By definition of A_{τ} , for all k -types $\tau_1, \tau_2 \in \Theta_k$ and all strings $s \in \Sigma^*$, $\tau_1 \rightsquigarrow^s \tau_2$ iff $\tau_1 \cdot \langle s \rangle_k = \tau_2$. Therefore as direct consequence of Proposition 1.3, there exists $m \geq 2^k$ such that $\tau_1 \rightsquigarrow^{s^m} \tau_2$ iff $\tau_1 \rightsquigarrow^{s^{m+1}} \tau_2$. In other words, the transition monoid of A_{τ} is aperiodic, and so is A_{τ} .

3 Aperiodic String Transducers

For sets A and B , we write $[A \rightarrow B]$ for the set of functions $F : A \rightarrow B$, and $[A \rightharpoonup B]$ for the set of partial functions $F : A \rightharpoonup B$. A string-to-string transformation from an input alphabet Σ to an output alphabet Γ is a partial function in $[\Sigma^* \rightharpoonup \Gamma^*]$. We have seen some examples of string-to-string transformations in the introduction. For the examples of first-order definable transformations we use the following representative example.

► **Example 5.** Let $\Sigma = \{a, b\}$. For all strings $s \in \Sigma^*$, we denote by \bar{s} its mirror image, and for all $\sigma \in \Sigma$, by $s \setminus \sigma$ the string obtained by removing all symbols σ from s . The transformation $f_1 : \Sigma^* \rightarrow \Sigma^*$ maps any string $s \in \Sigma^*$ to the output string $(s \setminus b) \bar{s} (s \setminus a)$. For example, $f_1(abaa) = aaa.aaba.b$.

3.1 First-order logic definable Transformations

Courcelle [11] initiated the study of structure transformations using monadic second-order logic. In this paper, we restrict this logic-based transformation model to FO-definable string transformations. The main idea of Courcelle's transformations is to define a transformation $(w, w') \in R$ by defining the string model of w' using a finite number of copies of positions of the string model of w . The existence of positions, various edges, and position labels are then given as FO(Σ) formulas.

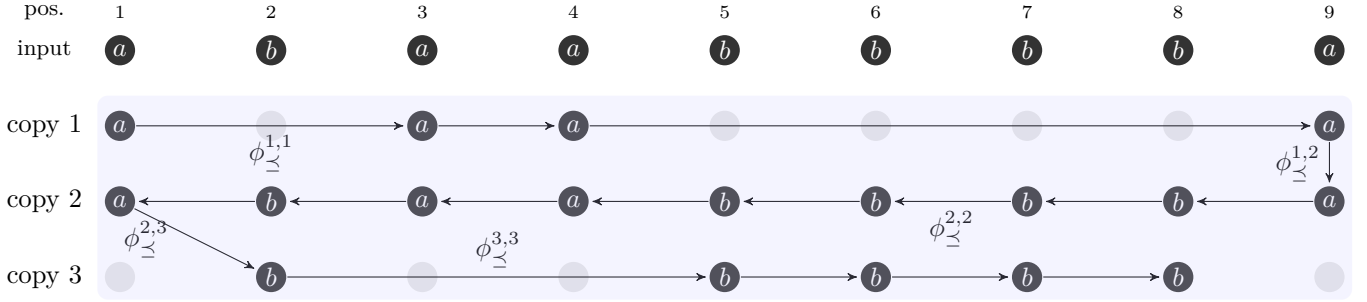
► **Definition 6 (First-order Transducers).** An *FO string transducer* is a tuple $T = (\Sigma, \Gamma, \phi_{\text{dom}}, C, \phi_{\text{pos}}, \phi_{\preceq})$ where:

- Σ and Γ are finite sets of input and output alphabets;
- ϕ_{dom} is a closed FO(Σ) formula characterizing the domain of the transformation;
- $C = \{1, 2, \dots, n\}$ is a finite index set;
- $\phi_{\text{pos}} = \{\phi_{\gamma}^c(x) : c \in C \text{ and } \gamma \in \Gamma\}$ is a finite set of FO(Σ) formulas with a free position variable x ;
- $\phi_{\preceq} = \{\phi_{\preceq}^{c,d}(x, y) : c, d \in C\}$ is a finite set of FO(Σ) formulas with two free position variables x and y .

The transformation $\llbracket T \rrbracket$ defined by T is as follows. A string s with $\Xi_s = (\text{dom}(s), \preceq, (L_a)_{a \in \Sigma})$ is in the domain of $\llbracket T \rrbracket$ if $s \models \phi_{\text{dom}}$ and the output is the relational structure $M = (D, \preceq^M, (L_{\gamma}^M)_{\gamma \in \Gamma})$ such that

- $D = \{v^c : c \in \text{dom}(s), c \in C \text{ and } \phi^c(v)\}$ is the set of positions where $\phi^c(v) \stackrel{\text{def}}{=} \bigvee_{\gamma \in \Gamma} \phi_{\gamma}^c(v)$;
- $\preceq^M \subseteq D \times D$ is the ordering relation between positions and it is such that for $v, u \in \text{dom}(s)$ and $c, d \in C$ we have that $v^c \preceq^M u^d$ if $w \models \phi_{\preceq}^{c,d}(v, u)$; and
- for all $v^c \in D$ we have that $L_{\gamma}^M(v^c)$ iff $\phi_{\gamma}^c(v)$.

Observe that the output is unique and therefore FO transducers implement functions. However, note that the output structure may not always be a string. We say that an FO transducer is a *string-to-string* transducer if its domain is restricted to string graphs and the output is also a string graph. We say that a string-to-string transformation is FO-definable if there exists an FO string-to-string transducer implementing the transformation. We write FOT for the set of FO-definable string-to-string transformations.



■ **Figure 2** First-Order Transduction $w \mapsto (w \setminus b) \bar{w} (w \setminus a)$

► **Example 7.** The best way, perhaps, to explain an FO transducers is via an example. Consider the transformation f_1 of Example 5. It can be defined using an FO transducer that uses three copies of the input domain, as illustrated on Fig. 2. The domain formula is $\phi_{\text{dom}} = \text{is_string}$. Intuitively, the first copy corresponds to $(w \setminus b)$, therefore the label formula $\phi_\gamma^1(x)$ is defined by false if $\gamma = b$ in order to filter out the input positions labelled b , and by true otherwise. For second copy corresponds to \bar{w} , hence all positions of the input are kept and their labels preserved (however the edge direction will be complemented) therefore the label formula is $\phi_\gamma^2(x) = L_\gamma(x)$. Finally, the third copy corresponds to $(w \setminus a)$ and hence $\phi_\gamma^3(x)$ is true if $\gamma = b$ and false otherwise. The transitive closure of the output successor relation is defined by:

$$\phi_{\leq}^{1,1}(x, y) = x \preceq y, \quad \phi_{\leq}^{2,2}(x, y) = y \preceq x, \quad \phi_{\leq}^{3,3}(x, y) = x \preceq y,$$

$$\phi_{\leq}^{c,c'}(x, y) = \text{true if } c < c', \phi_{\leq}^{c,c'}(x, y) = \text{false if } c' < c.$$

Note that the transitive closure is not depicted on the figure, but only the successor relation. Using first-order logic we define the position successor relation the following way: for all copies c, d , the existence of a direct edge from a position x^c to a position y^d of the output, also called the successor relation $S(x^c, y^d)$, is defined by the formula $\phi_{\text{succ}}^{c,d}(x, y) \stackrel{\text{def}}{=} \phi_{\leq}^{c,d}(x, y) \wedge \neg \exists z. \bigvee_{e \in C} \phi_{\leq}^{c,e}(x, z) \wedge \phi_{\leq}^{e,d}(z, y)$ where $\phi_{\leq}^{c_1,c_2}(x_1, x_2) \stackrel{\text{def}}{=} \phi_{\leq}^{c_1,c_2}(x_1, x_2) \wedge x_1 \neq x_2$ for all $c_1, c_2 \in C$.

We define the *quantifier rank* $qr(T)$ of an FOT T as the maximal quantifier rank of any formula in T , plus 1. We add 1 for technical reasons, mainly because defining the successor relation requires one quantifier.

3.2 Streaming String Transducers

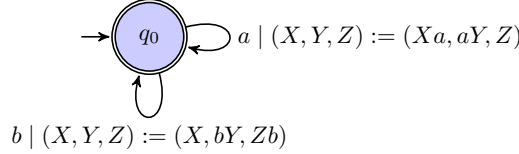
Streaming string transducers [1, 2] (SSTs) are one-way finite-state transducers that manipulates a finite set of string variables to compute its output. Instead of appending symbols to the output tape, SSTs concurrently update all string variables using a concatenation of string variables and output symbols. The transformation of a string is then defined using an output (partial) function F that associates states with a concatenation of string variables, s.t. if the state q is reached after reading the string and $F(q) = xy$, then the output string is the final valuation of x concatenated with that of y . In this section we formally introduce SSTs and introduce restrictions on SSTs that capture FO-definable transformations.

Let \mathcal{X} be a finite set of variables and Γ be a finite alphabet. A substitution σ is defined as a mapping $\sigma : \mathcal{X} \rightarrow (\Gamma \cup \mathcal{X})^*$. A valuation is defined as a substitution $\sigma : \mathcal{X} \rightarrow \Gamma^*$. Let $\mathcal{S}_{\mathcal{X}, \Gamma}$ be the set of all substitutions $[\mathcal{X} \rightarrow (\Gamma \cup \mathcal{X})^*]$. Any substitution σ can be extended to $\hat{\sigma} : (\Gamma \cup \mathcal{X})^* \rightarrow (\Gamma \cup \mathcal{X})^*$ in a straightforward manner. The composition $\sigma_1 \sigma_2$ of two substitutions σ_1 and σ_2 is defined as the standard function composition $\hat{\sigma}_1 \hat{\sigma}_2$, i.e. $\hat{\sigma}_1 \hat{\sigma}_2(X) = \hat{\sigma}_1(\hat{\sigma}_2(X))$ for all $X \in \mathcal{X}$. We are now in a position to introduce streaming string transducers.

► **Definition 8.** A deterministic streaming string transducer (SST) is a tuple $T = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ where:

- Σ and Γ are finite sets of input and output alphabets;
- Q is a finite set of states with initial state q_0 ;

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■ **Figure 3** SST implementing the transformation $s \mapsto (s \setminus b) \bar{s} (s \setminus a)$. Here the output function is $F(1) = XYZ$.

- $\delta : Q \times \Sigma \rightarrow Q$ is a transition function;
- \mathcal{X} is a finite set of variables;
- $\rho : \delta \rightarrow \mathcal{S}_{\mathcal{X}, \Gamma}$ is a variable update function;
- Q_f is a subset of final states;
- $F : Q_f \rightarrow \mathcal{X}^*$ is an output function.

The concept of a run of an SST is defined in an analogous manner to that of a finite state automaton. The sequence $\langle \sigma_{r,i} \rangle_{0 \leq i \leq |r|}$ of substitutions induced by a run $r = q_0 \xrightarrow{a_1} q_1 \xrightarrow{a_2} q_2 \dots q_{n-1} \xrightarrow{a_n} q_n$ is defined inductively as the following: $\sigma_{r,i} = \sigma_{r,i-1} \rho(q_{i-1}, a_i)$ for $1 < i \leq |r|$ and $\sigma_{r,1} = \rho(q_0, a_1)$. We denote $\sigma_{r,|r|}$ by σ_r .

If the run r is final, i.e. $q_n \in Q_f$, we can extend the output function F to the run r by $F(r) = \sigma_\epsilon \sigma_r F(q_n)$, where σ_ϵ substitute all variables by their initial value ϵ . For all strings $s \in \Sigma^*$, the output of s by T is defined only if there exists an accepting run r of T on s , and in that case the output is denoted by $T(s) = F(r)$. The transformation $\llbracket T \rrbracket$ defined by an SST T is the function $\{(s, T(s)) : T(s) \text{ is defined}\}$.

► **Example 9.** Let us consider the streaming string transducer T_2 shown in Figure 3 implementing the transformation f_1 introduced in Example 5. The SST T_2 has only one state q_0 , and three variables X, Y , and Z . The variable update is shown in the figure and the output function is s.t. $F(q_0) = XYZ$.

The following table shows a run of T_2 on the string $s = abaa$.

		a	b	a	a
X	ε	a	a	aa	aaa
Y	ε	a	ba	aba	$aaba$
Z	ε	ε	b	b	b

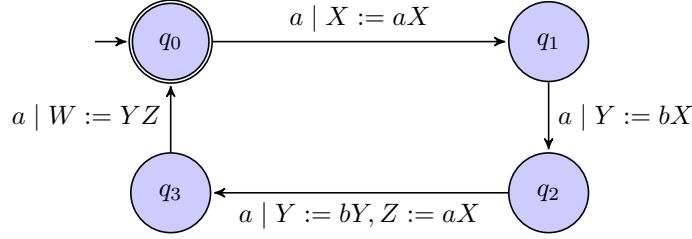
Let r be the run of T_2 on $s = abaa$. We have $\sigma_{r,1} : (X, Y, Z) \mapsto (Xa, aY, Z)$, $\sigma_{r,2} : (X, Y, Z) \mapsto \sigma_{r,1}(X, bY, Zb) = (Xa, baY, Zb)$, $\sigma_{r,3} : (X, Y, Z) \mapsto \sigma_{r,2}(Xa, aY, Z) = (Xaa, abaY, Zb)$ and $\sigma_{r,4} : (X, Y, Z) \mapsto \sigma_{r,3}(Xa, aY, Z) = (Xaaa, aabaY, Zb)$. Therefore $T(s) = F(r) = \sigma_\epsilon \sigma_{r,4} F(q_0) = \sigma_\epsilon \sigma_{r,4}(XYZ) = \sigma_\epsilon(XaaaabaYZb) = aaaaabab$.

3.3 Transition Monoid of Streaming String Transducers and Aperiodicity

We define the notion of aperiodic SSTs by introducing an appropriate notion of transition monoid for transducers. The transition monoid of an SST T is based on the effect of a string s on the states and variables. The effect on variables is characterized by, what we call, flow information that is given as a relation that describes the number of copies of the content of a given variable that contribute to another variable after reading a string s .

State and Variable Flow Let $T = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ be an SST. Let s be a string in Σ^* and suppose that there exists a run r of T on s . Recall that this run induces a substitution σ_r that maps each variable $X \in \mathcal{X}$ to a string $u \in (\Gamma \cup \mathcal{X})^*$. For string variables $X, Y \in \mathcal{X}$, states $p, q \in Q$, and $n \in \mathbb{N}$ we say that n copies of Y flow to X from p to q if there exists a run r on s from p to q , and Y occurs n times in $\sigma_r(X)$. We denote the flow with respect to a string s as $(p, Y) \rightsquigarrow_n^s (q, X)$.

► **Example 10.** Consider the run r from q_0 to q_0 over the string $aaaa$ in the following SST. While drawing an SST we often omit the update corresponding to the variables that retain their previous value.



On the run r on $aaaa$ can be seen that $\sigma_{r,4}(W) = \sigma_{r,3}[W := YZ] = \sigma_{r,3}(Y)\sigma_{r,3}(Z)$. However, $\sigma_{r,3}(Y) = b\sigma_{r,2}(Y) = b.b.\sigma_{r,1}(X)$ and $\sigma_{r,3}(Z) = a.\sigma_{r,2}(X) = a.\sigma_{r,1}(X)$, and $\sigma_{r,1}(X) = a$. Thus, on the run from q_0 to q_0 we have that $(q_0, Y) \rightsquigarrow_1^{aaaa} (q_0, W)$, $(q_0, Z) \rightsquigarrow_1^{aaaa} (q_0, W)$, $(q_0, X) \rightsquigarrow_2^{aaaa} (q_0, W)$.

Transition Monoid of an SST In order to define the transition monoid of an SST T , we first extend \mathbb{N} with an extra element \perp , and let $\mathbb{N}_\perp = \mathbb{N} \cup \{\perp\}$. This new element behaves as 0: for all $i \in \mathbb{N}_\perp$, $i.\perp = \perp.i = \perp$, $i + \perp = \perp + i = i$. Moreover, we assume that $\perp < n$ for all $n \in \mathbb{N}$. We assume that pairs $(p, X) \in Q \times \mathcal{X}$ are totally ordered. The *transition monoid* of T is the set of square matrices over \mathbb{N}_\perp indexed (in order) by elements of $Q \times \mathcal{X}$, defined by $M_T = \{M_s \mid s \in \Sigma^*\}$ where for all strings $s \in \Sigma^*$, $M_s[p, Y][q, X] = n \in \mathbb{N}$ iff $(p, Y) \rightsquigarrow_n^s (q, X)$, and $M_s[p, Y][q, X] = \perp$ iff there is no run from p to q on s . Note that, by definition, there is atmost one run r from (p, Y) to (q, X) on any string s .

It is easy to see that $(M_T, \times, \mathbf{1})$ is a monoid, where \times is defined as matrix multiplication and the identity element is the unit matrix $\mathbf{1}$. The mapping M_\bullet , which maps any string s to its transition matrix M_s , is a morphism from $(\Sigma^*, \cdot, \epsilon)$ to $(M_T, \times, \mathbf{1})$. We say that the transition monoid M_T of an SST T is n -bounded if all the coefficients of the matrices of M_T are bounded by n . Clearly, any n -bounded transition monoid is finite.

In [2], SST are required to have *copyless* updates, i.e., variable updates are defined by linear substitutions. In other words, the content of a variable can never flow into two different variables, and cannot flow more than once into another variable. In [3], this condition was slightly relaxed to the notion of *restricted copy*. This requirement imposes that a variable cannot flow more than once into another variable. This allows for a limited form of copy: for instance, X can flow to Y and Z , but Y and Z cannot flow to the same variable. Finally, *bounded copy* SSTs were introduced in [6] as a restriction on the variable dependency graphs. This restriction requires that there exists a bound K such that any variable flows at most K times in another variable. These three restrictions were shown to be equivalent, in the sense that SSTs with copyless, restricted copy, and bounded copy updates have the same expressive power. Given our definition of transition monoid, and the results of Alur, Filiot, and Trivedi [6], the following result is immediate by observing that bounded copy restriction of [6] for SSTs corresponds to finiteness of transition monoid. Also, notice that since the bounded copy assumption generalizes the copyless [2] and restricted copy [3] assumptions, previous definitions in the literature of streaming string transducers also correspond to finite transition monoids.

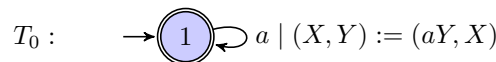
► **Theorem 11** ([6]). *A string transformation is MSO-definable iff it is definable by an SST with finite transition monoid.*

The main goal of this paper is to present a similar result for FO-definable transformations.

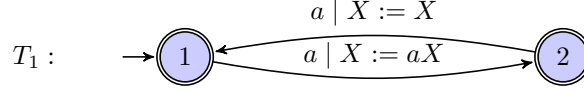
► **Definition 12** (Aperiodic SSTs). A streaming string transducer is aperiodic if its transition monoid is aperiodic.

► **Definition 13** (1-bounded SSTs). A streaming string transducer is 1-bounded if its transition monoid is 1-bounded. That is, for all strings s , and all pairs (p, Y) , (q, X) , $M_s[p, Y][q, X] \in \{\perp, 0, 1\}$.

► **Example 14.** (Aperiodic and non-aperiodic SSTs) Let us consider the transformation f_{halve} defined as $a^n \mapsto a^{\lceil \frac{n}{2} \rceil}$. Consider the SSTs T_1 with 2 states and 1 variable, and T_0 (its output is $F(1) = X$) both implementing f_{halve} .



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It can be seen that the transition monoids of both SSTs are 1-bounded but non aperiodic. In the first case this is caused by the variable flow, while in the second, this is caused by the transitions between states. The transition monoid of T_0 is a 2×2 matrix. For $k \geq 0$,

$$M_{a^{2k+1}} = \begin{matrix} & \begin{matrix} (1,X) & (1,Y) \end{matrix} \\ \begin{matrix} (1,X) \\ (1,Y) \end{matrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{matrix}, \quad M_{a^{2k}} = \begin{matrix} & \begin{matrix} (1,X) & (1,Y) \end{matrix} \\ \begin{matrix} (1,X) \\ (1,Y) \end{matrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{matrix}$$

The transition monoid of T_1 is a 2×2 matrix. For $k \geq 0$,

$$M_{a^{2k+1}} = \begin{matrix} & \begin{matrix} (1,X) & (2,X) \end{matrix} \\ \begin{matrix} (1,X) \\ (2,X) \end{matrix} & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{matrix}, \quad M_{a^{2k}} = \begin{matrix} & \begin{matrix} (1,X) & (2,X) \end{matrix} \\ \begin{matrix} (1,X) \\ (2,X) \end{matrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{matrix}$$

For both examples, we can see that there does not exist any $m \in \mathbb{N}$ such that $M_{a^m} = M_{a^{m+1}}$, thereby making both SSTs non aperiodic. On the other hand, for any string s , the transition monoid of the SST T_2 in Figure 3 is given by

$$M_s = \begin{matrix} & \begin{matrix} (1,X) & (1,Y) & (1,Z) \end{matrix} \\ \begin{matrix} (1,X) \\ (1,Y) \\ (1,Z) \end{matrix} & \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{matrix}$$

Clearly, M_{T_2} is aperiodic and 1-bounded.

The following result states that the domain of an aperiodic, 1-bounded SST is FO-definable.

► **Proposition 3.** The domain of an aperiodic SST is FO-definable.

Proof. Let $T = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ be an aperiodic SST and M_T its (aperiodic) transition monoid. Let us define a function φ which associates with each matrix $M \in M_T$, the $|Q| \times |Q|$ Boolean matrix $\varphi(M)$ defined by $\varphi(M)[p][q] = 1$ iff there exist $X, Y \in \mathcal{X}$ such that $M_T[p, X][q, Y] \geq 0$. Clearly, $\varphi(M_T)$ is the transition monoid of the underlying input automaton of T (ignoring the variable updates). The result follows, since the homomorphic image of an aperiodic monoid is aperiodic. ◀

We show that an SST is non-aperiodic iff its transition monoid contains a non-trivial cycle. Checking the existence of a non-trivial cycle has been shown to be in PSPACE for deterministic automata [17], but this result can be extended to our setting.

► **Lemma 15.** *Given an SST T , checking whether it is aperiodic and 1-bounded is PSPACE-COMplete.*

Proof. We first prove that given an SST T , checking whether its transition monoid M_T is 1-bounded is in PSPACE. We then show that checking whether a 1-bounded SST T is aperiodic is PSPACE-COMplete. The full proof can be seen in Appendix B.1. ◀

The rest of the paper is devoted to the proof of the following key theorem.

► **Theorem 16.** *A string transformation is FO-definable iff it is definable by an aperiodic, 1-bounded SST.*

The proof of this theorem follows from Lemma 19 (Section 5) and Lemma 17 (Section 4).

4 From aperiodic 1-bounded SST to FOT

In this section we show the following lemma by constructing an equivalent FOT T' for a given SST T .

► **Lemma 17.** *A string transformation is FO-definable if it is definable by an aperiodic, 1-bounded SST.*

The idea closely follows the SST-to-MSOT construction of [1, 6]. The main challenge here is to show that aperiodicity and 1-boundedness on the SST implies FO-definability of the output string structure (in particular the predicate \preceq).

4.1 FO-definability of variable flow

We first show that the variable flow of any aperiodic, 1-bounded SST is FO-definable. This will be crucial to show that the output predicate \preceq is FO-definable.

► **Proposition 4.** Let T be an aperiodic, 1-bounded SST T with set of variables \mathcal{X} . For all variables $X, Y \in \mathcal{X}$, there exists an FO-formula $\phi_{X \rightsquigarrow Y}(x, y)$ with two free variables such that, for all strings $s \in \text{dom}(T)$ and any two positions $i \leq j \in \text{dom}(s)$, $s \models \phi_{X \rightsquigarrow Y}(i, j)$ iff $(q_i, X) \rightsquigarrow_1^{s[i+1:j]} (q_j, Y)$, where $q_0 \dots q_n$ is the accepting run of T on s .

Let $X \in \mathcal{X}$, $s \in \text{dom}(T)$, $i \in \text{dom}(s)$, and let $n = |s|$. We say that the pair (X, i) is *useful* if the content of variable X before reading $s[i]$ will be part of the output after reading the whole string s . Formally, if $r = q_0 \dots q_n$ is the accepting run of T on s , then (X, i) is useful for s if $(q_{i-1}, X) \rightsquigarrow_1^{s[i:n]} (q_n, Y)$ for some variable $Y \in F(q_n)$. Thanks to Proposition 4, this property is FO-definable.

► **Proposition 5.** For all $X \in \mathcal{X}$, there exists an FO-formula $\text{useful}_X(i)$ s.t. for all strings $s \in \text{dom}(T)$ and all positions $i \in \text{dom}(s)$, $s \models \text{useful}_X(i)$ iff (X, i) is useful for string s .

Proofs of propositions 4 and 5 can be found in Appendix C.

4.2 SST-output relational structure

In this section, we define the SST-output structure given an input string structure. It is an intermediate representation of the output, and the transformation of any input string into its SST-output structure will be shown to be FO-definable.

For any SST T and string $s \in \text{dom}(T)$, the SST-output structure of s is a relational structure $G_T(s)$ obtained by taking, for each variable $X \in \mathcal{X}$, two copies of $\text{dom}(s)$, respectively denoted by X^{in} and X^{out} . For notational convenience we assume that these structures are labeled on the edges. This structure satisfies the following invariants: for all $i \in \text{dom}(s)$, (1) the nodes (X^{in}, i) and (X^{out}, i) exist only if (X, i) is useful, and (2) there is a directed path from (X^{in}, i) to (X^{out}, i) whose sequence of labels is equal to the value of the variable X computed by T after reading $s[i]$.

The condition on usefulness of nodes implies that SST-output structures consist of a single directed component, and therefore they are edge-labeled string structures.

As an example of SST-output structure consider Fig. 4. We show only the variable updates. Dashed arrows represent variable updates for useless variables, and therefore does not belong the SST-output structure. Initially the variable content of Z is equal to ϵ . It is represented by the ϵ -edge from $(Z^{\text{in}}, 0)$ to $(Z^{\text{out}}, 0)$ in the first column. Then, variable Z is updated to Zc . Therefore, the new content of Z starts with ϵ (represented by the ϵ -edge from $(Z^{\text{in}}, 1)$ to $(Z^{\text{out}}, 0)$, which is concatenated with the previous content of Z , and then concatenated with c (it is represented by the c -edge from $(Z^{\text{out}}, 0)$ to $(Z^{\text{out}}, 1)$). Note that the invariant is satisfied. The output is given by the path from $(X^{\text{in}}, 5)$ to $(X^{\text{out}}, 5)$ and equals $ceaeaaafbdcdcf$. Also note that some edges are labelled by strings with several letters, but there are finitely many possible such strings. In particular, we denote by O_T the set of all strings that appear in right-hand side of variable updates. SST-output structures are defined formally in Appendix C.3.

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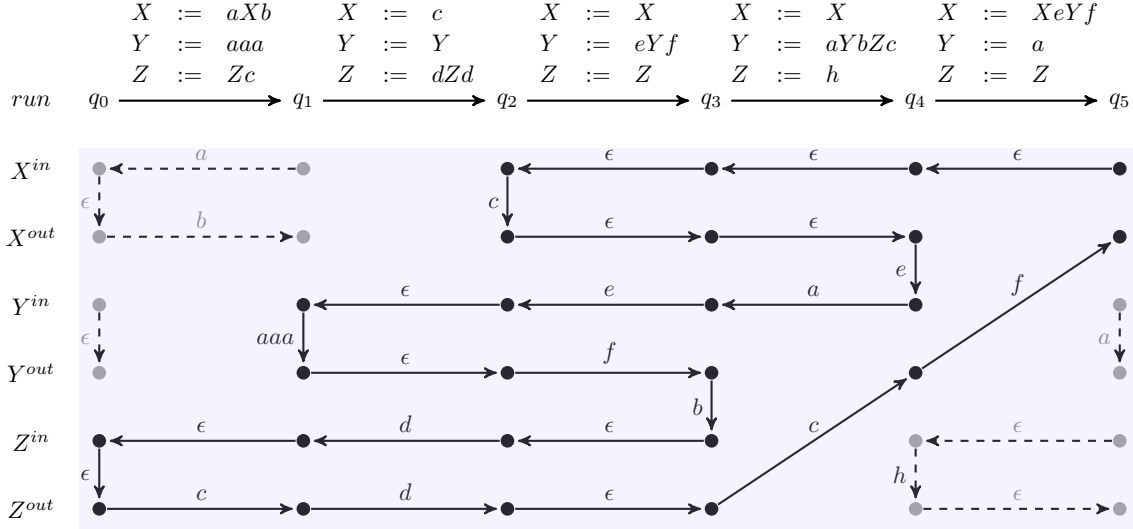


Figure 4 SST-output structure

4.3 From SST to FOT

It is known from [1, 6] that the transformation that maps a string s to its SST-output structure is MSO-definable. We show that it is FO-definable as long as the SST is aperiodic and 1-bounded. The main challenge is to define the transitive closure of the edge relation in first-order. We briefly recall the construction of [1, 6] in Appendix (in the proof of Lemma 17) but rather focus on the transitive closure in this section.

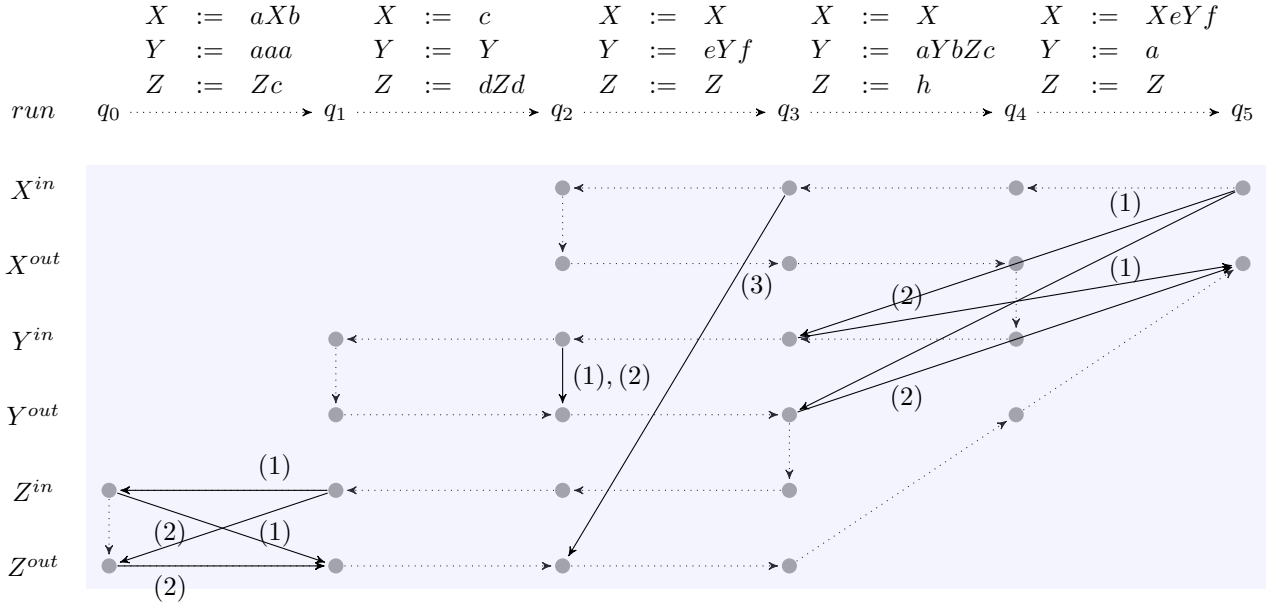
Let $T = (Q, q_0, \Sigma, \Gamma, \mathcal{X}, \delta, \rho, Q_f)$. The SST-output structure of T , as a node-labeled string, can be seen as logical structures over the signature $S_{O_T} = \{(E_\gamma)_{\gamma \in O_T}, \preceq\}$ where the symbols E_γ are binary predicates interpreted as edges labeled by O_T . We let E denote the edge relation, disregarding the labels. To prove that transitive closure is FO[Σ]-definable, we use the fact that variable flow is FO[Σ]-definable. The following property is a key result towards FO-definability.

► **Proposition 6.** Let T be an **aperiodic, 1-bounded** SST T . Let $s \in \text{dom}(T)$, $G_T(s)$ its SST-output structure and $r = q_0 \dots q_n$ the accepting run of T on s . For all variables $X, Y \in \mathcal{X}$, all positions $i, j \in \text{dom}(s) \cup \{0\}$, all $d, d' \in \{in, out\}$, there exists a path from node (X^d, i) to node $(Y^{d'}, j)$ in $G_T(s)$ iff (X, i) and (Y, j) are both useful and one of the following conditions hold: either

1. $(q_j, Y) \rightsquigarrow_1^{s[j+1:i]} (q_i, X)$ and $d = in$, or
2. $(q_i, X) \rightsquigarrow_1^{s[i+1:j]} (q_j, Y)$ and $d' = out$, or
3. there exists $k \geq \max(i, j)$ and two variables X', Y' such $(q_i, X) \rightsquigarrow_1^{s[i+1:k]} (q_k, X')$, $(q_j, Y) \rightsquigarrow_1^{s[j+1:k]} (q_k, Y')$ and X' and Y' are concatenated in this order¹ by r when reading $s[k+1]$.

We illustrate the conditions of this proposition on Fig.5. We have for instance $(q_2, Y) \rightsquigarrow_1^{s[3:2]=\epsilon} (q_2, Y)$, therefore by conditions (1) (and (2)) by taking $X = Y$ and $i = j = 2$, there exists a path from $(Y^{in}, 2)$ to $(Y^{out}, 2)$. Note that none of these conditions imply the existence of an edge from $(Y^{out}, 2)$ to $(Y^{in}, 2)$, but self-loops on $(Y^{in}, 2)$ and $(Y^{out}, 2)$ are implied by conditions (1) and (2) respectively. Now consider positions 0 and 1 and variable Z . It is the case that $(q_0, Z) \rightsquigarrow_1^{s[1:1]} (q_1, Z)$, therefore by condition (1) there is a path from $(Z^{in}, 1)$ to $(Z^{in}, 0)$ and to $(Z^{out}, 0)$. Similarly, by condition (2) there is a path from $(Z^{in}, 0)$ to $(Z^{out}, 1)$ and from $(Z^{out}, 0)$ to $(Z^{out}, 1)$. For positions 3 and 5, note that $(q_3, Y) \rightsquigarrow_1^{s[4:5]} (q_5, X)$, hence there is a path from $(Y^d, 3)$ to $(X^{out}, 5)$ for all $d \in \{in, out\}$. By condition (2) one also gets edges from $(X^{in}, 5)$ to $(Y^d, 3)$. Finally consider nodes $(Z^{out}, 2)$ and $(X^{in}, 3)$. There is no flow relation between variable Z at position 2 and variable X at position 3. However, $(q_3, X) \rightsquigarrow_1^{s[4:4]} (q_4, X)$ and

¹ by concatenated we mean that there exists a variable update whose rhs is of the form $\dots X' \dots Y' \dots$



■ **Figure 5** Conditions of Proposition 6

$(q_2, Z) \rightsquigarrow^{s[3:4]} (q_4, Y)$. Then X and Y gets concatenated at position 4 to define X at position 5. Therefore there is a path from $(X^{in}, 3)$ to $(Z^{out}, 2)$: this case is covered by condition (3).

From this result and FO-definability of variable flow, one can show that transitive closure is FO-definable.

► **Lemma 18.** *Let T be an **aperiodic, 1-bounded** SST T . For all $X, Y \in \mathcal{X}$ and all $d, d' \in \{in, out\}$, there exists an $FO[\Sigma]$ -formula $path_{X,Y,d,d'}(x, y)$ with two free variables such that for all strings $s \in \text{dom}(T)$ and all positions $i, j \in \text{dom}(s)$, $s \models path_{X,Y,d,d'}(i, j)$ iff there exists a path from (X^d, i) to $(Y^{d'}, j)$ in $G_T(s)$.*

The proof of Lemma 18 can be seen in Appendix D.1. We are now in a position to sketch the proof of Lemma 17 of this section. Let Γ be the output alphabet. The construction presented in [6, 1] shows the MSO-definability of strings to SST-output structures. We adapt this construction and based on FO-definability of transitive closure, as proved in Lemma 18, we show that strings to SST-output structure transformations are FO-definable whenever the SST is aperiodic and 1-bounded. In [6, 1], SST-output structures also contain useless nodes which are later on removed by composing another definable transformation. Based on Proposition 5 which states that usefulness of nodes is FO-definable, we rather directly filter out these nodes in the first FO-transformation. SST-output structures are however edge-labeled strings over O_T , where O_T is a finite set of strings over Γ . It remains to transform an edge-labeled string over O_T into a (node-labeled) string over Γ . This transformation is again FO-definable by taking a suitable number of copies of the input domain ($\max\{|s| \mid s \in O_T\}$). Then the lemma follows from the closure of FO-transformations under composition [11].

5 From FOT to aperiodic 1-bounded SST

The goal of this section is to prove the following lemma by showing a reduction from FO-definable transformations to aperiodic, 1-bounded SSTs.

► **Lemma 19.** *A string transformation is FO-definable only if it is definable by an aperiodic, 1-bounded SST.*

We begin this section by introducing the notion of aperiodic, 1-bounded SSTs with look-ahead, and show that they are equi-expressive to aperiodic, 1-bounded SSTs. We will then construct an aperiodic, 1-bounded SST with look-ahead

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implementing the same transformation as the given FOT. While this construction of the SST with look-ahead closely mimics the construction of [5], we show that it preserves aperiodicity and 1-boundedness (Section 5.3).

5.1 SSTs with Lookahead

As an intermediate model we introduce streaming string transducers with look-ahead (SST-la), which are SSTs that can make transitions based on some regular property of the current suffix of the input string. Such properties can be conveniently specified via a single finite automaton whose different states characterize various regular properties. Intuitively, while processing a symbol a_i of an input $w = a_1a_2 \dots a_n$, the SST moves from its current state to some state q_i iff there exists a unique state p_i of the look ahead automaton such that $a_ia_{i+1} \dots a_n \in L(p_i)$. As the string is processed, along with the current state of the SST, a set of states of the lookahead automaton is also maintained.

Formally, a (deterministic) lookahead automaton is a tuple $A = (Q_A, \Sigma, \delta_A, P_f)$ such that for all $p \in Q_A$ the tuple $A_p = (Q_A, p, \Sigma, \delta_A, P_f)$ (A with initial state p) is a deterministic finite automaton (we write $L(A_p)$ for the language that it recognizes).

► **Definition 20.** An SST with lookahead is a tuple (T, A) where $A = (Q_A, \Sigma, \delta_A, P_f)$ is a (deterministic) lookahead automaton and T is a tuple $(\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ where $\Sigma, \Gamma, Q, q_0, Q_f, \mathcal{X}, \rho$, and F are defined as for SSTs, and $\delta : Q \times \Sigma \times P \rightarrow Q$ is the transition function. We further require that the look-aheads are mutually exclusive, i.e. for all symbols $a \in \Sigma$, all states $q \in Q$, and all transitions $q' = \delta(q, a, p)$ and $q'' = \delta(q, a, p')$, we have that $L(A_p) \cap L(A_{p'}) = \emptyset$.

The requirement that look-aheads are mutually exclusive ensures that the SST-la is deterministic: when reading a new symbol, there is at most one transition that can be triggered. It is obvious that this requirement can be checked in polynomial time: whenever $q' = \delta(q, a, p)$ and $q'' = \delta(q, a, p')$, we can indeed construct a deterministic automaton \mathcal{A}_{mutex} which starts from the final states of A_p and $A_{p'}$ and walks backward to (p, p') such that $L(\mathcal{A}_{mutex}) = \emptyset$.

A configuration of an SST-la is a pair $(q_i, P_i) \in Q \times 2^P$. A run r of T over string $s = a_1 \dots a_n \in \Sigma^*$ is a sequence of configurations and letters $r = (q_0, P_0) \xrightarrow{a_1} (q_1, P_1) \dots (q_{n-1}, P_{n-1}) \xrightarrow{a_n} (q_n, P_n)$ such that for all $i \in \{0, \dots, n-1\}$, $(q_i, P_i) \xrightarrow{a_{i+1}} (q_{i+1}, P_{i+1})$ if there exists $p \in P_{i+1}$ such that $\delta(q_i, a_{i+1}, p) = q_{i+1}$, and for all $p \in P_i$, $\delta_A(p, a_{i+1}) \in P_{i+1}$. We write $(q_0, P_0) \rightsquigarrow^s (q_n, P_n)$ if such a sequence exists. We say that r is accepting if (q_0, P_0) is an initial configuration, i.e. $q_0 \in Q_0$ and $P_0 = \emptyset$, and (q_n, P_n) is an accepting configuration, i.e. $q_n \in Q_f$ and $P_n \subseteq P_f$. Clearly, if r is accepting, then for all $i \in \{1, \dots, n-1\}$, $a_{i+1} \dots a_n \in L(A_p)$, where p is the look-ahead state of the i -th transition of r . A configuration is said to be *accessible* if it can be reached from an initial configuration, and *co-accessible* if from it an accepting configuration can be reached. It is *useful* if it is both accessible and co-accessible. Note that from the mutual-exclusiveness of look-aheads and the determinism of A , it follows that for any input string, there is at most one run of the SST_{la} from and to useful configurations, as shown in Appendix E.

The concept of substitutions induced by a run can be naturally extended from SSTs to SST-las. Also, we can define the transformation implemented by an SST-la in a straightforward manner. The transition monoid of an SST-la is defined by matrices indexed by configurations $(q_i, P_i) \in Q \times 2^P$, using the notion of run defined before, and the definition of aperiodicity of SST-la follows that of SST. Adding look-aheads (in an aperiodic fashion) to SST does not increase their expressive power, see Appendix E.1.

► **Lemma 21.** *For all aperiodic, 1-bounded SST with look-ahead, there exists an equivalent aperiodic, 1-bounded SST.*

5.2 From FOT to SST with look-ahead

The main complication in showing this construction is that FO-transducers are *descriptive* i.e. they describe the function using logical formulas, while streaming string transducers are *computational* as they compute the output string by reading the input string in one left-to-right pass of the input string. Our goal is to construct an SST from an FO-transducer in such a way that after reading the string till the position i the variables in the SST will store the substrings of the output corresponding to positions up to index i in different variables, and to devise an update function for these variables to keep this invariant.

For instance, consider the FO-transduction shown in Figure 2 till position 3. Assume we omit the positions and edges of the output graph post position 3. Upto position 3, the output graph consists of two strings: the first string is between the positions 1^1 and 3^1 and stores aa , while the second string is between positions 3^2 and 2^3 and stores the string $abab$. Let us assume that these strings are stored in variables X_1 and X_2 , respectively. When we read the next letter of the string at position 4, we need to update these variables so as to append the letter a in the string stored in variable X_1 , while prepend the letter a to the string stored in variable X_2 using perhaps the following updates: $X_1 := X_1a$ and $X_2 := aX_2$. The next goal here is to identify the beginning (“ i -head”) and the ending (“ i -tails”) points of these output sub-string before the position i , and update them as we process the input string. In this section we show that these sub-strings can be uniquely identified using the k -types of a suitable decomposition of the input string.

Heads and tails of output substrings. We fix an FO transducer $T = (\Sigma, \Gamma, \phi_{\text{dom}}, C, \phi_{\text{pos}}, \phi_{\preceq})$ and let k be its quantifier rank. Let $s \in \Sigma^*$ and $j \in \text{dom}(s)$. For all copies $c \in C$, we denote by j^c the c th copy of the input j position, and say that j^c is *alive* if it contributes to the output string, i.e. there exists some $\gamma \in \Gamma$ such that $s \models \phi_{\gamma}^c(j)$. For instance, on Fig.2, alive positions are in bold. This can be defined in FO.

For $j \leq i \in \text{dom}(s)$, we call a position j^c an i -head if j^c is alive and there is no incoming edge to j^c that comes from some position l^d for some position $l \leq i$ and some $d \in C$. Formally, j^c is an i -head if $s \models \text{head}_c(i, j)$ where $\text{head}_c(x, y)$ is the following FO-formula:

$$\text{head}_c(x, y) \stackrel{\text{def}}{=} y \preceq x \wedge \text{alive}_c(y) \wedge \neg \exists z \cdot z \preceq x \wedge \bigvee_{d \in C} \text{alive}_d(z) \wedge \phi_{\text{succ}}^{d,c}(z, y)$$

where $\phi_{\text{succ}}^{d,c}(z, y)$ defines the (output) successor relation (it is FO-definable using $\Phi_{\preceq}^{d,c}$). The notion of i -tail can be defined similarly. Formally, j^c is an i -tail if $s \models \text{tail}_c(i, j)$ where $\text{tail}_c(x, y) = y \preceq x \wedge \text{alive}_c(y) \wedge \neg \exists z \cdot z \preceq x \wedge \bigvee_{d \in C} \text{alive}_d(z) \wedge \phi_{\text{succ}}^{d,c}(y, z)$.

The following lemma (proof in Appendix F.1) states for all strings s , all $i \in \text{dom}(s)$, an i -tail or an i -head, j^c , is uniquely determined by the k -type of the string $s[1:j]$, k -type of the string $s[j:i]$, k -type of the string $s(i:|s|]$, the symbol $s[j]$, and the corresponding copy c .

► **Lemma 22.** *Let $s \in \Sigma^*$, $i \in \text{dom}(s)$, $c \in C$, and $a \in \Sigma$. Let $j_1, j_2 \in \text{dom}(s)$. Then $j_1 = j_2$ if: (1) $j_1 < i$ and $j_2 < i$, (2) $s[j_1] = s[j_2] = a$, (3) $s[1:j_1] \equiv_{k+2} s[1:j_2]$, (4) $s(j_1:i] \equiv_{k+2} s(j_2:i]$, and (5) j_1^c and j_2^c are either both i -tails or both i -heads.*

As a corollary, the number of i -tails and i -heads is bounded by a constant that only depends on the transducer T .

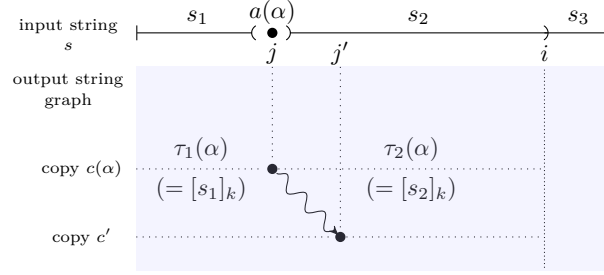
► **Corollary 23.** *For all $s \in \Sigma^*$, all $i \in \text{dom}(s)$ and $c \in C$, the number of i -tails and i -heads is bounded by $|\Theta_{k+2}|^2 \cdot |\Sigma| \cdot |C|$.*

Lemma 22 hints at a unique way to name a sub-string computed till position i by the unique address of its i -head j^c , as the tuple $(\langle s[1:j] \rangle_{k+2}, \langle s(j:i] \rangle_{k+2}, s[j], c)$. An *address* is defined as a tuple $\alpha \in \Theta_{k+2}^2 \times \Sigma \times C$. We denote by $\tau_1(\alpha)$, $\tau_2(\alpha)$, $a(\alpha)$, and $c(\alpha)$ the projections of α on the first, second, third, and fourth components, respectively. The set of addresses is denoted by \mathcal{A}_T .

As a consequence of Lemma 22, given a string $s \in \Sigma^*$ and a position $i \in \text{dom}(s)$, any address $\alpha \in \mathcal{A}_T$ defines at most one i -tail or i -head in s . The head $\text{HD}(s, i, \alpha)$ of an address $\alpha \in \mathcal{A}_T$ at position i in some input string $s \in \Sigma^*$ is the position $(j, c) \in \text{dom}(s) \times C$ in the output structure s.t. $s \models \text{head}_c(i, j)$, $\tau_1(\alpha) = \langle s[1:j] \rangle_{k+2}$, $a(\alpha) = s[j]$, $\tau_2(\alpha) = \langle s(j:i] \rangle_{k+2}$, and $c(\alpha) = c$ (By Lemma 22, (j, c) is indeed unique). If these conditions are not satisfied, then we say that $\text{HD}(s, i, \alpha)$ is undefined. Similarly, the tail $\text{TL}(s, i, \alpha)$ of an address $\alpha \in \mathcal{A}_T$ at position i in $s \in \Sigma^*$ is defined if (i) there exists some (j', c') such that $(j', c') = \text{HD}(s, i, \alpha)$ is defined, and (ii) $\text{TL}(s, i, \alpha)$ is the position $(j, c) \in \text{dom}(s) \times C$ in the output structure such that $s \models \text{tail}_c(i, j) \wedge \phi_{\preceq}^{c',c}(j', j)$, and for all $c'' \in C$, all $j'' > i$, $s \not\models \phi_{\preceq}^{c',c''}(j', j'') \wedge \phi_{\preceq}^{c'',c}(j'', j)$ (i.e. the path from (j', c') to (j, c) only consists of positions (j'', c'') such that $j'' \leq i$).

Fig. 6 illustrates the notions of i -head and i -tail of an address. It represents an output position $j^{c(\alpha)}$ which is the head of the address $\alpha \in \mathcal{A}_T$ at position i in string s . The input string s is decomposed as $s = s_1(a(\alpha))s_2s_3$ such

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■ **Figure 6** Head $\text{HD}(s, i, \alpha) = (j, c(\alpha))$ and tail $\text{TL}(s, i, \alpha) = (j', c')$ for an address $\alpha \in \mathcal{A}_T$.

that $[s_1]_k = \tau_1(\alpha)$ and $[s_2]_k = \tau_2(\alpha)$. From the definition it is clear that the heads and the tails of addresses are FO-definable. The proof of Lemma 24 can be found in Appendix F.2.

► **Lemma 24.** *The functions HD and TL are FO-definable, i.e. given $\alpha \in \mathcal{A}_T$ and a copy $c \in C$, there exist two FO-formula $\Phi_{\text{HD}(\alpha)}^c(x, y)$ (of quantifier rank at most $k + 2$) and $\Phi_{\text{TL}(\alpha)}^c(x, y)$ (of quantifier rank at most $k + 3$) such that for all $s \in \Sigma^*$ and $i, j \in \text{dom}(s)$, $s \models \Phi_{\text{HD}(\alpha)}^c(i, j)$ iff $\text{HD}(s, i, \alpha)$ is defined and $\text{HD}(s, i, \alpha) = (j, c)$, and, $s \models \Phi_{\text{TL}(\alpha)}^c(i, j)$ iff $\text{TL}(s, i, \alpha)$ is defined and $\text{TL}(s, i, \alpha) = (j, c)$.*

SST Construction

Given an FOT, to obtain the corresponding SST, we define the set of SST variables $\mathcal{X} = \{X_\alpha : \alpha \in \mathcal{A}_T\}$. While reading a string, we will maintain the invariant that after reading the position i of the input string s , the variable X_α will store the output substring rooted at position $j^c = \text{HD}(s, i, \alpha)$ iff j^c is an i -head, otherwise the variable X_α will contain ϵ .

The next challenge is to show how to update these string variables. There are several cases to consider depending on the new direct edges in the output graph from some copy in the current position to a head or a tail of a variable relative to the previous position, or vice-versa. In general, for a variable X_α we have an update rule $X_\alpha = \gamma X_{\alpha_1} \gamma_1 X_{\alpha_2} \dots X_{\alpha_n} \gamma_n$ such that $|\gamma X_{\alpha_1} \gamma_1 X_{\alpha_2} \dots X_{\alpha_n} \gamma_n| \leq |C|$. Thus, there are only a bounded number of updates to consider. Given a string and a position $i \in \text{dom}(s)$ we can write an FO-formula $\Phi_{\text{upd}}[X_\alpha := \gamma X_{\alpha_1} \gamma_1 X_{\alpha_2} \dots X_{\alpha_n} \gamma_n](i)$ of quantifier rank at most $k + 5$ which characterizes the update corresponding to the current position. We briefly sketch some update formulas. For instance,

1. $s \models \Phi_{\text{upd}}[X_\alpha := \epsilon](i)$ if $\text{HD}(s, i, \alpha)$ is not defined;
2. $s \models \Phi_{\text{upd}}[X_\alpha := X_{\alpha'}](i)$ if both $\text{HD}(s, i, \alpha)$ and $\text{HD}(s, i-1, \alpha')$ are defined and are equal to each-other and $\text{TL}(s, i, \alpha) = \text{TL}(s, i-1, \alpha')$;
3. $s \models \Phi_{\text{upd}}[X_\alpha := \gamma X_{\alpha'} \gamma' X_{\alpha''} \gamma''](i)$ if $\text{HD}(s, i, \alpha)$ is defined, both $\text{HD}(s, i-1, \alpha')$ and $\text{HD}(s, i-1, \alpha'')$ are defined, $\tau_2(\alpha) = \langle \epsilon \rangle_k$ and there is an edge in the output structure from $i^{c(\alpha)}$ to $\text{HD}(s, i-1, \alpha')$, the label of the node $i^{c(\alpha)}$ is γ , there is a copy c' such that the position $i^{c'}$ is labeled γ' and $i^{c'}$ has a direct edge from $\text{TL}(s, i-1, \alpha')$ and $i^{c'}$ has a direct edge to $\text{HD}(s, i-1, \alpha'')$, and there is copy c'' such that the position $i^{c''}$ is labeled γ'' and has a direct edge from $\text{TL}(s, i-1, \alpha'')$. By reusing variable names, we have to use only 2 nested extra quantifiers to express this formula, and therefore, since any formula $\Phi_{\text{TL}(\alpha)}^c$ has quantifier rank at most $k + 3$, we can express this variable update by a formula of quantifier rank at most $k + 5$. This variable update easily generalizes to longer concatenations of variables, while using formulas of quantifier rank at most $k + 5$ only.

We also define the look-around formula $\Phi_{\tau, a, \tau'}(i)$ that holds for a string s if the substring $s[1:i] \models \Phi_\tau$, the substring $s(i:|s|) \models \Phi_{\tau'}$ and $s[i] = a$.

Now we are in a position to construct an equivalent SST-la (T_{la}, A) from a given FOT $T = (\Sigma, \Gamma, \phi_{\text{dom}}, C, \phi_{\text{pos}}, \phi_{\leq})$. Let $T_{\text{la}} = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ be a look-ahead SST with look-ahead $A = (Q_A, \Sigma, \delta_A, P_f)$. The look-ahead automaton $A = (Q_A, \Sigma, \delta_A, P_f)$ is constructed as a collection of automata that capture FO sentence Φ_τ for all

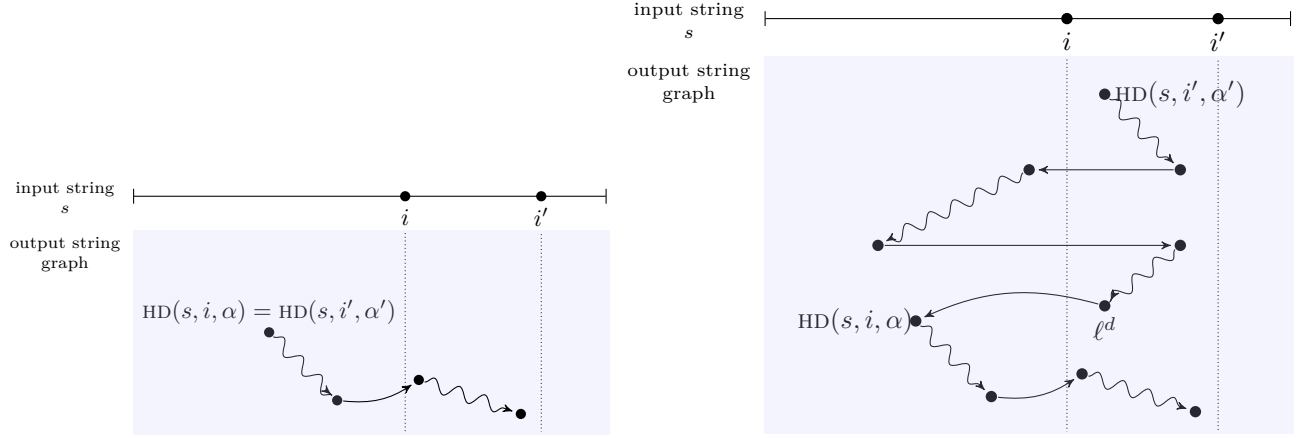


Figure 7 Variable flow information is FO-definable.

$\tau \in \Theta_{k+2}$. More precisely, $A = \bigcup_{\tau \in \Theta_{k+2}} A_\tau$ where A_τ is the automaton accepting strings of type τ as introduced in Sec. 2. For convenience we assume that the states of A are pairs (τ, τ') where τ corresponds to the FO type that is checked and τ' is a state of A_τ , and write $p_\tau \in Q_A$ for the state $(\tau, \langle \epsilon \rangle_{k+2}) \in Q_A$. In particular, the set of strings s such that $\langle s \rangle_{k+2} = \tau$ equals $L(A_{p_\tau})$. The SST T_{la} is a tuple $(\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ where

- the set of states is the set of $k+2$ types, i.e. $Q = \Theta_{k+2}$;
- the initial state is $q_0 = \langle \epsilon \rangle_{k+2}$;
- the set of final states are the $(k+2)$ -types that implies the domain formula ϕ_{dom} (on strings), i.e. $Q_f = \{\tau : \tau \models \phi_{\text{dom}}\}$;
- the transition function $\delta : Q \times \Sigma \times Q_A \rightarrow Q$ is defined such that $\delta(\tau, a, p_{\tau'}) = \tau''$ where $\tau'' = \tau.\langle a \rangle_k$;
- the set of variables is defined as $\mathcal{X} = \{X_\alpha : \alpha \in \mathcal{A}_T\}$;
- the output function is simply the concatenation of all the variables since after reading the whole string only a unique address is alive, i.e. all the variables except the variable corresponding to that address must be empty, i.e. $F(q) = \prod_{X \in \mathcal{X}} X$; and
- the update function $\rho : \delta \rightarrow \mathcal{S}_{\mathcal{X}, \Gamma}$ is defined by $\rho(\tau, a, p_{\tau'})(X_\alpha) := \gamma X_{\alpha_1} \gamma_1 X_{\alpha_2} \gamma_2 \dots X_{\alpha_n} \gamma_n$ if $n \leq C$ and the following formula is valid (on strings, which is decidable): $\forall x. (\Phi_{\tau, a, \tau'}(x) \rightarrow \Phi_{\text{upd}}[X_\alpha := \gamma X_{\alpha_1} \gamma_1 X_{\alpha_2} \gamma_2 \dots X_{\alpha_n} \gamma_n](x))$.

5.3 Aperiodicity and 1-boundedness of SST-la

In this section, we first prove that the SST_{la} $T_{\text{la}} = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ with look-ahead $A = (Q_A, \Sigma, \delta_A, P_f)$ constructed in the previous section is aperiodic and 1-bounded, i.e., its transition monoid is aperiodic and 1-bounded. Given a tuple $t = (q, q', R, R', X_\alpha, X_{\alpha'}, m) \in Q^2 \times (2^{Q_A})^2 \times \mathcal{X} \times \mathbb{N}$, we show that the flow is FO-definable, i.e. there exists an FO-sentence flow_t such that for all strings $s \in \Sigma^*$, $s \models \text{flow}_t$ iff $((q, R), X_\alpha) \rightsquigarrow_m^s ((q', R'), X_{\alpha'})$. Then, aperiodicity of the transition monoid of T will follow by Proposition 1.3. Indeed, we know that there exists n_0 such that for all strings $s \in \Sigma^*$, $s^{n_0} \equiv_b s^{n_0+1}$ and therefore, $s^{n_0} \models \text{flow}_t$ iff $s^{n_0+1} \models \text{flow}_t$, where b is quantifier rank of the formulas flow_t . We start with the following observation: for all strings $s \in \text{dom}(T_{\text{la}})$, there exists exactly one accepting run of T_{la} on s (proved in Appendix G.1). We first prove a result on the state flow of T_{la} .

► **Lemma 25.** (State Flow) *Given two states $q, q' \in Q$, and two sets $R, R' \in 2^{Q_A}$. There exists an FO-formula $\text{sflow}_{q, q', R, R'}(x, y)$ of quantifier rank at most $k+3$ such that for all strings $s \in \text{dom}(T_{\text{la}})$ of length $n \geq 1$ and any two positions $i, i' \in \text{dom}(s)$, $s \models \text{sflow}_{q, q', R, R'}(i, i')$ iff $i \leq i'$ and the (unique accepting) run $r = (q_0, R_0) \dots (q_n, R_n)$ of T_{la} on s satisfies $(q_{i-1}, R_{i-1}) = (q, R)$ and $(q_{i'}, R_{i'}) = (q', R')$.*

Proof (Sketch). By definition of T_{la} and its look-ahead automaton, we precisely characterize the configurations (q_j, R_j) in FO. For instance, the fact that the main run of T_{la} is in q at position x , by definition of T_{la} , is equivalent to say that the prefix up to x has type q (remind that $Q = \Theta_k$). It is expressible in FO by a formula with one

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free variable x obtained by guarding all quantifiers of any variable z in Φ_τ by $z \preceq x$, where Φ_τ has been defined in Prop. 2. The full proof is in Appendix G.2. \blacktriangleleft

The flow between variables is characterized by the following property.

► **Lemma 26.** (*Variable Flow*) Let $X_\alpha, X_{\alpha'} \in \mathcal{X}$ be two variables, $s \in \text{dom}(T_{\text{la}})$ a string of length $n \geq 1$ and $i \leq i' \in \text{dom}(s)$ two positions of s . Let $r = (q_0, R_0) \dots (q_n, R_n)$ be the accepting run of T_{la} on s . Then $(q_{i-1}, R_{i-1}, X_\alpha) \rightsquigarrow_m^{s[i:i']}(q_{i'}, R_{i'}, X_{\alpha'})$ for some $m \geq 1$ iff (1) $\text{HD}(s, i, \alpha)$ and $\text{HD}(s, i', \alpha')$ are both defined; (2) there is a path from $\text{HD}(s, i', \alpha')$ to $\text{HD}(s, i, \alpha)$ such that each node (j'', c'') of this path is such that $j'' \leq i'$. Formally, if $\text{HD}(s, i, \alpha) = (j, c)$ and $\text{HD}(s, i', \alpha') = (j', c')$, then $s \models \phi_{\preceq}^{c', c}(j', j)$ and, for all $c'' \in C$ and all $j'' \leq |s|$, if $s \models \phi_{\preceq}^{c', c''}(j', j'') \wedge \phi_{\preceq}^{c'', c}(j'', j)$, then $j'' \leq i'$. Moreover, $(q_{i-1}, R_{i-1}, X_\alpha) \rightsquigarrow_m^{s[i:i']}(q_{i'}, R_{i'}, X_{\alpha'})$ for some $m \geq 1$ iff $(q_{i-1}, R_{i-1}, X_\alpha) \rightsquigarrow_1^{s[i:i']}(q_{i'}, R_{i'}, X_{\alpha'})$.

Proof (Sketch). Suppose that all the conditions are met (the converse is proved similarly). Consider first the particular case where $\text{HD}(s, i, \alpha) = \text{HD}(s, i', \alpha')$ depicted in left-side of Figure 7. It means that the output node $\text{HD}(s, i, \alpha)$ is both an i -head and an i' -head. The name of this node however has changed to $\text{HD}(s, i', \alpha')$ at position i' , and possibly, the path represented by variable X_α at position i has been extended (as shown on the figure). By construction of T_{la} , variable X_α at position i flows into variable $X_{\alpha'}$ at position i' through the sequence of variable updates $X_{\alpha_j} := X_{\alpha_{j-1}}$ for all $i \leq j \leq i'$ where $\alpha_i = \alpha$ and $\alpha_{i'} = \alpha'$, and for all $i \leq j \leq i'$, $a(\alpha_j) = a_j$ (the j -th symbol of s), $\tau_1(\alpha_j) = \tau_1(\alpha_{j-1}) \cdot [a_j]_k$, $\tau_2(\alpha_j) = [s[j..i']]_k$ and $c(\alpha_j) = c(\alpha)$.

The other case is when the node $\text{HD}(s, i, \alpha)$ is the target of an edge from some (alive) node ℓ^d such that $i < \ell \leq i'$, i.e., $\text{HD}(s, i, \alpha)$ is an i -head but is not an i' -head. This new position ℓ^d belongs to some path that never goes beyond position i' , and the i' -head of this path is represented, by construction of T_{la} , by some variable. If this variable is precisely $X_{\alpha'}$, then one gets that X_α at position i flows into $X_{\alpha'}$ at position i' , by construction of variable update in T_{la} . It is depicted in right-side of Figure 7. On the figure, the path from node $\text{HD}(s, i', \alpha')$ contains node $\text{HD}(s, i, \alpha)$. Therefore the content of variable $X_{\alpha'}$ at position i' depends on the content of variable X_α at position i .

From this characterization of variable flow, it is easy to see that a variable cannot flow multiple times to another variable, since there exists only one path from $\text{HD}(s, i', \alpha')$ to $\text{HD}(s, i, \alpha)$. \blacktriangleleft

Based on the two previous lemmas, we are now able to express the “relative” flow of states and variables of T_{la} in between two positions of a string $s \in \text{dom}(T_{\text{la}})$ in FO.

► **Lemma 27.** (*Relative State-Variable Flow*) Given a tuple $t = (q, q', R, R', X_\alpha, X'_\alpha, m) \in Q \times Q \times 2^{Q_A} \times 2^{Q_A} \times \mathcal{X} \times \mathcal{X} \times \mathbb{N}$, there exists an FO-formula $\text{rflow}_t(x, y)$ of quantifier rank at most $k + 4$ such that for all strings $s \in \text{dom}(T_{\text{la}})$ of length $n \geq 1$ and any two positions $i \leq i' \in \text{dom}(s)$, if $r = (q_0, R_0) \dots (q_n, R_n)$ is the accepting run of T_{la} on s , then $s \models \text{rflow}_t(i, i')$ iff $(q_{i-1}, R_{i-1}, X_\alpha) \rightsquigarrow_m^{s[i:i']}(q_{i'}, R_{i'}, X_{\alpha'})$ for some $m \geq 1$. Moreover, $(q_{i-1}, R_{i-1}, X_\alpha) \rightsquigarrow_m^{s[i:i']}(q_{i'}, R_{i'}, X_{\alpha'})$ for some $m \geq 1$ iff $(q_{i-1}, R_{i-1}, X_\alpha) \rightsquigarrow_1^{s[i:i']}(q_{i'}, R_{i'}, X_{\alpha'})$.

Proof. We express the conditions of Lemma 26 in FO and take the resulting formula in conjunction with the formula $\text{sflow}_{q, q', R, R'}(x, y)$ obtained from Lemma 25. The full proof is in Appendix G.3. \blacktriangleleft

The formulas $\text{rflow}_t(x, y)$ for tuples $t = (q, q', R, R', X_\alpha, X'_\alpha, m)$ describe the flow between two positions x and y of some string $s \in \text{dom}(T_{\text{la}})$, with respect to the unique run of T_{la} on s . However to prove aperiodicity of the transition monoid of T_{la} , one has to express the flow on a whole string s (which is not necessarily in $\text{dom}(T_{\text{la}})$), and this flow must only depend on the starting and ending configurations (q, R) and (q', R') resp. In particular, (q, R, X_α) flows to (q', R', X'_α) on s is not equivalent to $s \models \text{rflow}_t(1, n)$ where $n = |s|$, because the run of T_{la} on s may not start with (q, R) . However, the flow of an SST with look-ahead is defined between useful configurations only, i.e. configurations which are both accessible from an initial state and co-accessible (a final state is accessible from them). Thanks to this requirement, we are able to express the flow on a string by using $\text{rflow}_t(x, y)$. This formula is first transformed into an aperiodic automaton that runs on strings extended with boolean values that indicate the positions of x and y . Then we take the quotient of this automaton to define the set of substrings from position x to position y and project the boolean values away. All these steps preserve aperiodicity. A proof of Lemma 28 can be found in Appendix G.4.

► **Lemma 28.** *Given a tuple $t = (q, q', R, R', X_\alpha, X'_\alpha, m) \in Q \times Q \times 2^{Q_A} \times 2^{Q_A} \times \mathcal{X} \times \mathcal{X} \times \mathbb{N}$ such that (q, R) and (q', R') are both useful, there exists an FO-sentence flow_t of quantifier rank at most $k + 4$ such that for all strings $s \in \Sigma^*$ and any two positions $i < i' \in \text{dom}(s)$, $s \models \text{flow}_t$ iff $(q, R, X_\alpha) \rightsquigarrow_m^s (q', R', X'_\alpha)$ for some $m \geq 1$. Moreover, $(q, R, X_\alpha) \rightsquigarrow_m^s (q', R', X'_\alpha)$ for some $m \geq 1$ iff $(q, R, X_\alpha) \rightsquigarrow_1^s (q', R', X'_\alpha)$.*

Sketch of Proof. The proof of this result is based on automata. The formula $\text{rflow}_t(x, y)$ is transformed into an aperiodic automaton A_1 that runs on strings extended with Boolean values that indicate the positions x and y . This automaton can be modified into an automaton A_2 that accepts only factors of strings s accepted by A_1 from position x to position y , while preserving aperiodicity. The automaton A_2 is then projected on alphabet Σ , getting an aperiodic automaton A_3 . Then the sentence flow_t is defined as an FO-sentence equivalent to A_3 . Usefulness of (q, R) and (q', R') is needed to ensure that (q, R, X_α) s -flows in (q', R', X'_α) implies $s \models \text{flow}_t$. Indeed, in that case, there exist two strings s_1, s_2 and the accepting run of T_{la} on $s_1 s s_2$ reaches (q, R) after reading s_1 and (q', R') after reading $s_1 s$ and therefore, $s_1 s s_2 \models \text{rflow}_t(|s_1| + 1, |s_1| + |s|)$ by Lemma 27, from which we can prove that $s \models \text{flow}_t$. ◀

► **Corollary 29.** *The $\text{SST}_{la} T_{la}$ is aperiodic and 1-bounded.*

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A

 Proofs from Section 2.3

A.1 Proof of Proposition 1.2

Proof. We prove the proposition for formulas with two free variables. The case of one free variable is a particular case. The proof is based on the composition result of Proposition 1.1.

Let $s = s_1 a s_2 b s_3$ and $s' = s'_1 a s'_2 b s'_3$. Considering the extended alphabet $\Sigma' = \Sigma \times \{0, 1\}^2$, we define the string $u = u_1 \begin{pmatrix} a \\ 1 \\ 0 \end{pmatrix} u_2 \begin{pmatrix} b \\ 0 \\ 1 \end{pmatrix} u_3$ where $u_i \in \left\{ \begin{pmatrix} c \\ 0 \\ 0 \end{pmatrix} \mid c \in \Sigma \right\}^*$. u is an extension of s (hence u_i is an extension of s_i). The two extra bits serve as the interpretation of first order variables x, y with $x = 1$ at position i_1 and $y = 1$ at position i_2 . In a similar manner, we define u' as well as u'_i as extensions of s' and s'_i respectively.

Since $s_i \equiv_{k+2} s'_i$ for all $i \in \{1, 2, 3\}$, we obtain $u_i \equiv_{k+2} u'_i$ by extending the signature of FO to $\Sigma \times \{0, 1\}^2$. Therefore by Proposition 1.1, we get $u \equiv_{k+2} u'$. Replacing every atomic formula $L_\gamma(z)$ of $\phi(x, y)$ by $\bigvee_{m,n \in \{0,1\}} L_{\begin{pmatrix} \gamma \\ m \\ n \end{pmatrix}}(z)$, we obtain the formula $\phi'(x, y)$. Quantifying x, y we obtain the sentence $\psi_{xy} = \exists x \exists y \bigvee_{c,d \in \Sigma} L_{\begin{pmatrix} c \\ 1 \\ 0 \end{pmatrix}}(x) \wedge L_{\begin{pmatrix} d \\ 0 \\ 1 \end{pmatrix}}(y) \wedge \phi'(x, y)$. It can be easily checked that $s \models \phi(i_1, i_2)$ iff $u \models \psi_{xy}$ and $s' \models \phi(i'_1, i'_2)$ iff $u' \models \psi_{xy}$. Since the quantifier rank of ϕ is at most k , the quantifier rank of ψ_{xy} is at most $k + 2$. Since $u \equiv_{k+2} u'$, we get $s \models \phi(i_1, i_2)$ iff $u \models \psi_{xy}$ iff $u' \models \psi_{xy}$ iff $s' \models \phi(i'_1, i'_2)$. \blacktriangleleft

B

 Proofs from Section 3.3

B.1 Proof of Lemma 15

► **Lemma 30.** *Given an SST T , checking whether its transition monoid M_T is 1-bounded is in PSPACE.*

Proof. Let $T = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$ be an SST. To check if T is 1-bounded, we have to check that there does not exist a string $s = s_1 s_2$ having a run from some state p to state q such that

- There is a run on string s_1 from state p to state r , such that variable X 1-flows into variables Y, Z .
- There is a run on string s_2 from state r to state q such that, variables Y, Z 1-flow into variable G

Clearly, if the above situation happens, X 2-flows into variable G , and $M_{s_1}[(p, X)][(r, Y)] = 1 = M_{s_1}[(p, X)][(r, Z)]$, $M_{s_2}[(r, Y)][(q, G)] = 1 = M_{s_2}[(r, Z)][(q, G)]$, and hence $M_s[(p, X)][(q, G)] = 2$, which means T is not 1-bounded. We give below, the algorithm to check if T is 1-bounded.

1. Successively guess the symbols of two strings s_1 and s_2 and along the way, keep computing the transition matrices M_{s_1} and M_{s_2} . This is possible to be done in PSPACE.
2. Compute $M_{s_1} \times M_{s_2}$ and check if it contains an integer $i \geq 2$. If so, then as discussed above, there is a variable X that i -flows into some variable G .

Clearly, the overall complexity of this algorithm is NPSpace. Thanks to Savitch's Theorem, we have a PSPACE algorithm. \blacktriangleleft

► **Lemma 31.** *Checking whether a given 1-bounded SST is aperiodic is PSPACE-COMplete.*

Proof. Given an SST $T = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$, we first construct an automaton A_T such that the transition monoids of T and A_T are the same. By definition, T is aperiodic iff its transition monoid M_T is aperiodic. It is known [10] that a deterministic (not necessarily minimal) finite state automaton is non-aperiodic iff there is some string $u \in \Sigma^*$ with the “non-trivial cycle property”. We cannot directly apply this result of [10] to A_T since in general, A_T could be non-deterministic. However, we show that M_T is non-aperiodic iff there exists a non-trivial cycle in A_T (note that this result is in general not true for arbitrary automata: for instance, one can have an automaton A accepting the aperiodic language $(ab)^*$; however the transition monoid of A could be non-aperiodic).

Given an automaton, we explain what the “non-trivial cycle property” means: There is a string u and a state p such $p \notin \delta(p, u)$, and for some positive integer r , $p \in \delta(p, u^r)$. In this proof, we show that M_{A_T} is non-aperiodic iff there is a string $u \in \Sigma^*$ that has the “non-trivial cycle property” in A_T .

First, we explain the construction of A_T from T . Given T , A_T is constructed as $(Q \times \mathcal{X}, \Sigma, \delta_A, q_0 \times \mathcal{X}, Q_f \times \mathcal{X})$ where $\delta((p, X), a) = \{(q, Y) \mid \text{there is a transition from } p \text{ to } q \text{ on } a, \text{ such that on the variable update on this transition, } X \text{ flows to } Y\}$. Corresponding to one transition from p to q on a in T , we have the transitions from (p, X_i) to (q, X_j) on a in A_T , whenever variable X_j is updated and X_i flows into X_j on that update. It is easy to see that the transition monoids of T , A_T are same.

Suppose now that there exists a non-trivial cycle in A_T . Then, there exists a string u and a state (p, X) and $m \geq 0$ such that $M_u[(p, X)][(p, X)] = 0$, and $M_{u^m}[(p, X)][(p, X)] = 1$. We want to show that M_T is not aperiodic. That is, there exists some string v such that, for all k , $M_{v^k} \neq M_{v^{k+1}}$.

Let $k \geq 0$. We show that $M_{u^k}[(p, X)][(p, X)] = 1$ implies $M_{u^{k+1}}[(p, X)][(p, X)] = 0$.

1. If $k = 0$, this is trivially true, since $M_\epsilon[(p, X)][(p, X)] = 1$ and $M_u[(p, X)][(p, X)] = 0$.
2. If $k > 0$, then assume that $M_{u^k}[(p, X)][(p, X)] = 1$. We show that $M_{u^{k+1}}[(p, X)][(p, X)] = 0$. Therefore suppose that $M_{u^{k+1}}[(p, X)][(p, X)] = 1$ and we will arrive at a contradiction.

By assumption, $M_u[(p, X)][(p, X)] = 0$. Since we also assume $M_{u^{k+1}}[(p, X)][(p, X)] = 1$, it is necessarily the case that $M_{u^k}[(p, X)][(q, Y)] = 1$ and $M_u[(q, Y)][(p, X)] = 1$ for some $(q, Y) \neq (p, X)$. Since the underlying SST T is deterministic and p is reachable from p on u^k (since $M_{u^k}[(p, X)][(p, X)] = 1$), we necessarily have that $q = p$. Therefore $X \neq Y$. Now, we have the situation depicted in Figure 8. Clearly, this contradicts the 1-boundedness of the SST. Therefore, we get $M_{u^{k+1}}[(p, X)][(p, X)] = 0$.

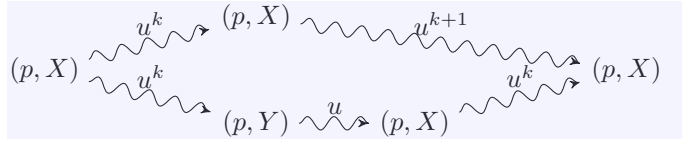


Figure 8 Multiple paths in A_T : X flows into X and Y on u^k ; further on u^{k+1} , X flows into X , and Y flows into X . This gives $(p, X) \rightsquigarrow_2^w (p, X)$, for $w = u^{2k+1}$, contradicting 1-boundedness.

It cannot be the case that T is aperiodic : If it were, then there exists m_0 such that for all $n \geq m_0$ we have $M_{u^n} = M_{u^{n+1}}$. We know that $M_{u^m}[(p, X)][(p, X)] = 1$, therefore $M_{u^{i.m}}[(p, X)][(p, X)] = 1$ for all i . Take i such that $i.m \geq m_0$. Then $M_{u^{i.m}}[(p, X)][(p, X)] = M_{u^{i.m+1}}[(p, X)][(p, X)] = 1$. This however, contradicts what we just showed i.e., $M_{u^k}[(p, X)][(p, X)] = 1 \Rightarrow M_{u^{k+1}}[(p, X)][(p, X)] = 0$.

Conversely, assume that M_T is not aperiodic. Then there is a string u such that for all m , $M_{u^m} \neq M_{u^{m+1}}$. We show the existence of a non-trivial cycle in A_T .

Assume now that, for all states (p, X) , and for all $m \geq 1$, and all strings u , $M_{u^m}[(p, X)][(p, X)] = 1$ iff $M_u[(p, X)][(p, X)] = 1$. Note that this is the same as saying that all strings u give rise only to trivial cycles. We will arrive at a contradiction to this assumption. By non-aperiodicity, we can pick some large m for which $M_{u^m} \neq M_{u^{m+1}}$. Then there are states (p, X) and (q, Y) such that $M_{u^m}[(p, X)][(q, Y)] \neq M_{u^{m+1}}[(p, X)][(q, Y)]$.

1. Without loss of generality, assume $M_{u^m}[(p, X)][(q, Y)] = 1$. If we take $m > |Q| \cdot |\mathcal{X}|$, then on the run of u^m from (p, X) to (q, Y) in A_T , we will revisit a state (r, Z) more than once. Assume that the run is such that $(p, X) \rightsquigarrow^{u^{l_1}} (r, Z) \rightsquigarrow^{u^{l_2}} (r, Z) \rightsquigarrow^{u^{l_3}} (q, Y)$ where $l_1 + l_2 + l_3 = m$. By our assumption on “only trivial cycles”, we know that $M_u[(r, Z)][(r, Z)] = 1$ since $M_{u^{l_2}}[(r, Z)][(r, Z)] = 1$. Hence, we also have the run $(p, X) \rightsquigarrow^{u^{l_1}} (r, Z) \rightsquigarrow^{u^{l_2+1}} (r, Z) \rightsquigarrow^{u^{l_3}} (q, Y)$ in A_T . This gives $M_{u^{m+1}}[(p, X)][(q, Y)] = 1$, contradicting our assumption of $M_{u^m}[(p, X)][(q, Y)] \neq M_{u^{m+1}}[(p, X)][(q, Y)]$.
2. Consider the case $M_{u^m}[(p, X)][(q, Y)] = 0$. We now consider the run in A_T from (p, X) to (q, Y) on u^{m+1} , where (r, Z) is revisited on u^l for some $l > 0$. Again, the “only trivial cycles” assumption then gives us a run on u^m from (p, X) to (q, Y) contradicting $M_{u^m}[(p, X)][(q, Y)] \neq M_{u^{m+1}}[(p, X)][(q, Y)]$.

Thus, we have shown that M_T is aperiodic iff all strings satisfy the trivial cycle property in A_T . It remains now to check the existence of a string u having the non-trivial cycle property in A_T . Adapting Stern's algorithm [17] to non-deterministic automata, we show that checking the existence of a string u having the non-trivial cycle property can be done in PSPACE. Briefly, we successively guess the symbols of a string u and compute the transition matrix of u . Next, we guess a state (p, X) . From the transition matrix of u , we can check if $M_u[(p, X)][(p, X)] = 0$. If so, we guess an integer $r \leq |Q \times \mathcal{X}|$ and compute M_{u^r} . If $M_{u^r}[(p, X)][(p, X)] = 1$, then we have found a non-trivial cycle. Using the PSPACE-hardness of checking non-trivial cycles in [10], we conclude that checking aperiodicity of SSTs is PSPACE-complete. ◀

C Proofs from Section 4.1

C.1 Proof of Proposition 4

First, we show that states of accepting runs of aperiodic SST are FO-definable:

► **Proposition 7.** Let T be an aperiodic SST T . For all states q , there exists an FO-formula $\phi_q(x)$ such that for all strings $s \in \Sigma^+$, for all positions i , $s \models \phi_q(i)$ iff $s \in \text{dom}(T)$ and the state of the (unique) accepting run of T before reading the i -th symbol of s is q . There exists an FO-sentence ϕ_q^{last} that defines the last state of the accepting run of T on s (if it exists).

Proof. Let A be the underlying (deterministic) automaton of T . Since T is aperiodic, so is A . For all q , let L_q be the set of strings s such that there exists a run of T on s that ends in q . Clearly, L_q can be defined by some aperiodic automaton A_q obtained by setting the set of final states of A to $\{q\}$. Therefore L_q is definable by some FO-formula ψ_q^L . Let R_q be the set of strings s such that there exists a run of T on s from q to some accepting state. Clearly, $u \in \text{dom}(T)$ iff there exists $q \in Q$, $v \in L_q$ and $w \in R_q$ such that $u = vw$. The language R_q is also definable by the aperiodic automaton obtained by setting the initial state of A to q , and therefore is definable by some FO-formula ψ_q^R .

Then, $\phi_q(x)$ is defined as

$$\phi_q(x) = [\psi_q^L]_{\prec x} \wedge [\psi_q^R]_{x \preceq}$$

where $[\psi_q^L]_{\prec x}$ is the formula ψ_q^L in which all quantifications of any variable y is guarded by $y \prec x$ and, similarly, $[\psi_q^R]_{x \preceq}$ is the formula ψ_q^R in which all quantifications of any variable y is guarded by $x \preceq y$. Therefore, $s \models \phi_q(i)$ iff $s[1:i] \in L_q$ and $s[i:|s|] \in R_q$.

The formula ϕ_q^{last} is constructed similarly. ◀

Now we start the proof of Proposition 4.

Proof. For all states $p, q \in Q$, let $L_{(p,X) \rightsquigarrow (q,Y)}$ be the language of strings u such that $(p, X) \rightsquigarrow_1^u (q, Y)$. We show that $L_{(p,X) \rightsquigarrow (q,Y)}$ is an aperiodic language. It is indeed definable by an aperiodic non-deterministic automaton A that keeps track of flow information when reading u . It is constructed from T as follows. Its state set Q' are pairs $(r, Z) \in 2^{Q \times \mathcal{X}}$. Its initial state is $\{(p, X)\}$ and final states are all states P such that $(q, Y) \in P$. There exists a transition $P \xrightarrow{a} P'$ in A iff for all $(p_2, X_2) \in P'$, there exists $(p_1, X_1) \in P$ and a transition $p_1 \xrightarrow{a|\rho} p_2$ in T such that $\rho(X_2)$ contains an occurrence of X_1 . Note that by definition of A , there exists a run from a state P to a state P' on some $s \in \Sigma^*$ iff for all $(p_2, X_2) \in P'$, there exists $(p_1, X_1) \in P$ such that $(p_1, X_1) \rightsquigarrow_1^s (p_2, X_2)$ (Remark \star).

Clearly, $L(A) = L_{(p,X) \rightsquigarrow (q,Y)}$. It remains to show that A is aperiodic, i.e. its transition monoid M_A is aperiodic. Since T is aperiodic, there exists $m \geq 0$ such that for all matrices $M \in M_T$, $M^m = M^{m+1}$. For $s \in \Sigma^*$, let $\Phi_A(s) \in M_A$ (resp. $\Phi_T(s)$) the square matrix of dimension $|Q'|$ (resp. $|Q|$) associated with s in M_A (resp. in M_T). We show that $\Phi_A(s^m) = \Phi_A(s^{m+1})$, i.e. $(P, P') \in \Phi_A(s^m)$ iff $(P, P') \in \Phi_A(s^{m+1})$, for all $P, P' \in Q'$.

First, suppose that $(P, P') \in \Phi_A(s^m)$, and let $(p_2, X_2) \in P'$. By definition of A , there exists $(p_1, X_1) \in P$ such that $(p_1, X_1) \rightsquigarrow_1^{s^m} (p_2, X_2)$, and by aperiodicity of T , it implies that $(p_1, X_1) \rightsquigarrow_1^{s^{m+1}} (p_2, X_2)$. Since it is true for all $(p_2, X_2) \in P'$, it implies by Remark (\star) that there exists a run of A from P to P' on s^{m+1} , i.e. $(P, P') \in \Phi_A(s^{m+1})$. The converse is proved similarly.

We have just proved that $L_{(p,X) \rightsquigarrow (q,Y)}$ is aperiodic. Therefore it is definable by some FO-formula $\phi_{(p,X) \rightsquigarrow (q,Y)}$. Now, $\phi_{X \rightsquigarrow Y}(x, y)$ is defined by

$$\phi_{X \rightsquigarrow Y}(x, y) \equiv x \preceq y \wedge \bigvee_{p, q \in Q} \{ [\phi_{(p,X) \rightsquigarrow (q,Y)}]^{x \preceq \cdot \preceq y} \wedge \phi_p(x) \wedge ((\text{last}(y) \rightarrow \phi_q^{\text{last}}) \wedge (\neg \text{last}(y) \rightarrow \bigvee_{r \in Q} \phi_r(y+1))) \},$$

where ϕ_p , ϕ_r and ϕ_q^{last} were defined in Proposition 7 and $[\phi_{(p,X) \rightsquigarrow (q,Y)}]^{x \preceq \cdot \preceq y}$ is obtained from $\phi_{(p,X) \rightsquigarrow (q,Y)}$ by guarding all the quantifications of any variable z by $x \preceq z \preceq y$. ◀

C.2 Proof of Proposition 5

Proof. The formula $\text{useful}_X(x)$ is defined by

$$\text{useful}_X(x) = \exists y \cdot \text{last}(y) \wedge \bigwedge_{p \in Q, q \in Q_f} (\Phi_q^{\text{last}} \rightarrow \bigvee_{Y \in F(q)} \Phi_p(x) \wedge \Phi_{X \rightsquigarrow Y}(x, y))$$

where $\text{last}(y)$ defines the last position of the string, $\Phi_p(x)$ is defined in proposition 7 and $\Phi_{X \rightsquigarrow Y}(x, y)$ in proposition 4. ◀

C.3 Definition of SST-output graphs

Let $T = (Q, q_0, \Sigma, \Gamma, \mathcal{X}, \delta, \rho, Q_f)$ be an SST. Let $u \in (\Gamma \cup X)^*$ and $s \in \Gamma^*$. The string s is said to *occur* in u if s is a factor of u . In particular, ϵ occurs in u for all u . Let O_T be the set of constant strings occurring in variable updates, i.e. $O_T = \{s \in \Gamma^* \mid \exists t \in \delta, s \text{ occurs in } \rho(t)\}$. Note that O_T is finite since δ is finite.

Let $s \in \text{dom}(T)$. The SST-output graph of s by T , denoted by $G_T(s)$, is defined as a directed graph whose edges are labelled by elements of O_T . Formally, it is the graph $G_T(s) = (V, (E_\gamma)_{\gamma \in O_T})$ where $V = \{0, 1, \dots, |w|\} \times \mathcal{X} \times \{\text{in}, \text{out}\}$ is the set of vertices, $E := \bigcup_{\gamma \in O_T} E_\gamma \subseteq V \times V$ is the set of labelled edges defined as follows.

Vertices $(i, X, d) \in V$ are denoted by (X^d, i) . Let $n = |s|$ and $r = q_0 \dots q_n$ the accepting run of T on s . The set E is defined as the smallest set such that for all $X \in \mathcal{X}$,

1. $((X^{\text{in}}, 0), (X^{\text{out}}, 0)) \in E_\epsilon$ if $(X, 0)$ is useful,
2. for all $i < n$ and $X \in \mathcal{X}$, if (X, i) is useful and if $\rho(q_i, s[i+1], q_{i+1})(X) = \gamma$, then $((X^{\text{in}}, i+1), (X^{\text{out}}, i+1)) \in E_\gamma$,
3. for all $i < n$ and $X \in \mathcal{X}$, if (X, i) is useful and if $\rho(q_i, s[i+1], q_{i+1})(X) = \gamma_1 X_1 \dots \gamma_k X_k \gamma_{k+1}$ (with $k > 1$), then
 - $((X^{\text{in}}, i+1), (X_1^{\text{in}}, i)) \in E_{\gamma_1}$
 - $((X_k^{\text{out}}, i), (X^{\text{out}}, i+1)) \in E_{\gamma_{k+1}}$
 - for all $1 \leq j < k$, $((X_j^{\text{out}}, i), (X_{j+1}^{\text{in}}, i)) \in E_{\gamma_{j+1}}$

Note that since the transition monoid of T is 1-bounded, it is never the case that two copies of some variable (say X) flows into some variable (say Y), therefore this graph is well-defined and there is **no** multiple edges between two nodes.

D Proofs fom Section 4.3

► Proposition 8. $G_T(s)$ consists of a unique directed path. Moreover, the concatenation of edge labels occurring along this path equals $T(s)$.

D.1 Proof of Lemma 18

Proof. For all variables $X, Y \in \mathcal{X}$, we denote by $C_{X,Y}$ the set of pairs $(p, q, a) \in Q^2 \times \Sigma$ such that there exists a transition from p to q on a whose variable update concatenate X and Y (in this order). We first define a formula for condition (3):

$$\Psi_3^{X,Y}(x, y) \equiv \exists z \cdot x \preceq z \wedge y \preceq z \wedge \bigvee_{X', Y' \in \mathcal{X}, (p, q, a) \in C_{X', Y'}} [L_a(z) \wedge \phi_{X \rightsquigarrow X'}(x, z) \wedge \phi_{Y \rightsquigarrow Y'}(y, z) \wedge \phi_p(z) \wedge \phi_q(z+1)]$$

Then, formula $\text{path}_{X,Y,d,d'}(x,y)$ is defined by

$$\begin{aligned} \text{path}_{X,Y,in,in}(x,y) &\equiv \phi_{Y \rightsquigarrow X}(y,x) \vee \Psi_3^{X,Y} \\ \text{path}_{X,Y,in,out}(x,y) &\equiv \phi_{Y \rightsquigarrow X}(y,x) \vee \phi_{X \rightsquigarrow Y}(x,y) \vee \Psi_3^{X,Y} \\ \text{path}_{X,Y,out,in}(x,y) &\equiv \text{false} \\ \text{path}_{X,Y,out,out}(x,y) &\equiv \phi_{X \rightsquigarrow Y}(x,y) \vee \Psi_3^{X,Y} \end{aligned}$$

◀

D.2 Proof of Lemma 17

We show here that the transformation which associates a string s with its SST-output graph $G_T(s)$ is FO-definable whenever T is aperiodic and 1-bounded, based on Lemma 18 and the construction of [6, 1]. The idea of [6, 1] is to define the accepting runs of T by using set variables, as for classical automata-to-MSO transformations, and to use state information in order to determine which variable updates apply and then define the edge relations. There is a copy of the domain for each variable x and each $d \in \{in, out\}$. Since states, variable flow and paths are all FO-definable when T is aperiodic and 1-bounded, it follows that G_T is FOT-definable. We refer the reader to [6, 1] for more details, but we recall here that the domain formula ϕ_{dom} is a sentence defining the domain of T , and therefore in our case is FO-definable, since $\text{dom}(T)$ is aperiodic. To illustrate the construction, we also give the formula $\phi_{E_\gamma}^{X^{in}, X^{in}}(y,x)$ that defines the γ -labelled edge relation for the domain copy X^{in} . It is defined by

$$y = x + 1 \wedge \bigvee_{t:=(p,a,q) \in \delta, \rho(t)(X)=\gamma X\beta \dots} L_a(y) \wedge \phi_p(x) \wedge \phi_q(y) \wedge \text{useful}_X(y)$$

where ϕ_p and ϕ_q are FO-formulas defined in proposition 7 and $\text{useful}_X(y)$ has been defined in Proposition 5.

Thanks to Lemma 18, the transitive closure between some copy X^d and some copy $Y^{d'}$ is defined by the FO-formula

$$\phi_{\preceq}^{X^d, Y^{d'}}(x,y) \equiv \text{path}_{X,Y,d,d'}(x,y)$$

◀

E Proofs from Section 5.1

We first define the transition monoid of an SST-la (T, A) where $A = (Q_A, \Sigma, \delta_A, P_f)$ is a deterministic lookahead automaton and $T = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$.

Uniqueness of accepting runs Let $s = s_1 \dots s_n \in \Sigma^*$ and $r : (q_0, P_0) \xrightarrow{s_1} (q_1, P_1) \dots (q_{n-1}, P_{n-1}) \xrightarrow{s_n} (q_n, P_n)$ be an accepting run of (T, A) on s . We not only show that r is unique, but that the sequence of transitions associated with r is unique. Given a sequence of transitions of T , it is clear that there exists exactly one run associated with that sequence, since A is deterministic.

Suppose the sequence of transitions is not unique, i.e. there exists another accepting run on r which follows another transition of T eventually. Let $i \geq 1$ be the smallest index where the i -th transitions are different on both runs. Before taking the i -th transition, both runs are in the configuration (q_{i-1}, P_{i-1}) . Suppose that the i -th transition on the first run is (q_{i-1}, a, p, q_i) for some look-ahead state p , and is (q_{i-1}, a, p', q'_i) on the other run, for some state q'_i and look-ahead state p' such that either $p \neq p'$ or $q_i \neq q'_i$. Since both runs are accepting, the suffix $s_{i+1} \dots s_n$ is in $L(A_p) \cap L(A_{p'})$, which is impossible by the mutual-exclusiveness of look-aheads. Therefore $p = p'$, but in that case, $q_i = q'_i$ since δ is a function. This leads to a contradiction.

Variable Flow and Transition Monoid for SST-la. Let Q_A represent the states of the (deterministic) lookahead automaton A , and Q denote states of the SST-la.

The transition monoid of an SST with look-ahead depends on its configurations and variables. It extends the notion of transition monoid for SST with look-ahead states components but is defined only on *useful* configurations

(q, P) . A configuration (q, P) is *useful* iff it is *accessible* and *co-accessible* : that is, (q, P) is reachable from the initial configuration (q_0, \emptyset) and some accepting configuration $(q_f, P) \in Q_f \times 2^{P_f}$ is reachable from (q, P) .

Note that given two useful configurations (q, P) , (q', P') and a string $s \in \Sigma^*$, there exists at most one run from (q, P) to (q', P') on s . Indeed, since (q, P) and (q', P') are both useful, there exists $s_1, s_2 \in \Sigma^*$ such that $(q_0, \emptyset) \rightsquigarrow^{s_1} (q, P)$ and $(q', P') \rightsquigarrow^{s_2} (q_f, R_f)$ where (q_f, R_f) is accepting. If there are two runs from (q, P) to (q', P') on s , then we can construct two accepting runs on $s_1 s s_2$, which contradicts the fact that accepting runs are unique. We can even strengthen this result by showing that the sequence of transitions associated with the unique run from (q, P) to (q', P') on s is as well unique. We denote by $\text{useful}(T, A)$ the useful configurations of (T, A) .

Thanks to the uniqueness of the sequence of transitions associated with the run of an SST-la from and to useful configurations on a given string, one can extend the notion of variable flow naturally by considering, as for SST, the composition of the variable updates along the run.

A string $s \in \Sigma^*$ maps to a square matrix M_s of dimension $|Q \times 2^{Q_A}| \cdot |\mathcal{X}|$ and is defined by $M_s[(q, P), X][(q', P'), X'] = n$ if there exists a run r from (q, P) to (q', P') on s such that n copies of X flows to X' over the run r , and (q, P) and (q', P') are both useful (which implies that the sequence of transitions of r from (q, P) to (q', P') is unique, as seen before), otherwise $M_s[(q, P), X][(q', P'), X'] = \perp$.

E.1 Proof of Lemma 21

Proof. Let (T, A) be an SST_{la}, with $A = (Q_A, \Sigma, \delta_A, P_f)$ a deterministic lookahead automaton, and $T = (\Sigma, \Gamma, Q, q_0, Q_f, \delta, \mathcal{X}, \rho, F)$. Without loss of generality, we make the following assumption

Assumption \star : $\forall q, q', q'' \in Q, \forall p, p' \in Q_A, \forall a \in \Sigma, \quad p \neq p' \wedge \delta(q, a, p) = q' \wedge \delta(q, a, p') = q'' \implies q' \neq q''$

This is indeed wlog: if (T, A) does not satisfy this assumption, then we can have as many copies of states Q as states of Q_A (i.e. the new set of states of T is $Q \times Q_A$) and transform the transitions accordingly to maintain uniqueness of the successor states w.r.t. to input symbols and look-ahead states. Moreover, it is easy to show that this transformation preserves aperiodicity.

Construction of T' We construct an aperiodic and 1-bounded SST T' equivalent to T . As explained in definition 20, the unique run of a string s on (T, A) is not only a sequence of Q -states, but also a collection of the look ahead states 2^{Q_A} . At any time, the current state of Q , and collection of look-ahead states $P \subseteq Q_A$ is a configuration. A configuration (q_1, P_1) , on reading a , evolves into $(q_2, P_2 \cup \{p_2\})$, where $\delta(q_1, a, p_2) = q_2$ is a transition in the SST-la and $\delta_A(P_1, a) = P_2$, where δ_A is the transition function of the look ahead automaton A . Note that the transition monoid of the SST-la is aperiodic and 1-bounded by assumption. We now show how to remove the look-ahead, resulting in an equivalent SST T' whose transition monoid is aperiodic and 1-bounded.

While defining T' , we “collect” together all the states resulting from transitions of the form (q, a, p, q') and (q, a, p', q'') in the SST-la. We define $T' = (\Sigma, \Gamma, Q', q'_0, \delta', \mathcal{X}', \rho', Q'_f)$ with:

- $Q' = 2^{\text{useful}(T, A)}$ where $\text{useful}(T, A)$ are the useful configurations of (T, A) ($\text{useful}(T, A)$ is computable in exponential time from (T, A)),
- $q'_0 = \{(q_0, \emptyset)\}$ (wlog we assume that (T, A) accepts at least one input therefore (q_0, \emptyset) is useful),
- Q'_f , the set of accepting states, is defined by $\{S \in Q' \mid \exists (q, P) \in S, q \in Q_f \wedge P \subseteq P_f\}$.
- $\mathcal{X}' = \{X_{q'} \mid X \in \mathcal{X}, q' \in \text{useful}(T, A)\}$,
- The transitions are defined as follows: $\delta'(S, a) = \bigcup_{(q, P) \in S} \Delta((q, P), a)$ where $\Delta((q, P), a) = \{(q', P' \cup \{p'\}) \mid (q, a, p', q') \in \delta \text{ and } \delta_A(P, a) = P'\} \cap \text{useful}(T, A)$.

Before defining the update function, we first assume a total ordering $\preceq_{\text{useful}(T, A)}$ on $\text{useful}(T, A)$. For all $(p, P) \in Q \times 2^{Q_A}$, we define the substitution $\sigma_{(p, P)}$ as $X \in \mathcal{X} \mapsto X_{(p, P)}$. Let (S, a, S') be a transition of T' . Given a state (q', P') in S' , there might be several predecessor states $(q_1, P_1), \dots, (q_k, P_k)$ in S on reading a . The set $\{(q_1, P_k), \dots, (q_k, P_k)\} \subseteq S$ is denoted by $\text{Pres}((q', P'), a)$. Formally, it is defined by $\{(q, P) \in S \mid (q', P') \in \Delta((q, P), a)\}$.

We consider only the variable update of the transition from the minimal predecessor state. Indeed, since any string has at most one accepting run in the SST-la (T, A) (and at most one associated sequence of transitions), if two runs

reach the same state at some point, they will anyway define the same output and therefore we can drop one of the variable update, as shown in [6]. Formally, the variable update $\rho'(S, a, S')(X_{(q', P')})$, for all $X_{(q', P')} \in \mathcal{X}'$ is defined by ϵ if $(q', P') \notin S'$, and by $\sigma_{(q, P)} \circ \rho(q, a, p, q')(X)$, where $(q, P) = \min \{(r, R) \in S \mid (q', P') \in \Delta((r, R), a)\}$, and $\delta(q, a, p) = q'$ (by Assumption \star the look-ahead state p is unique). It is shown in [6] that indeed T' is equivalent to T . We show here that the transition monoid of T' is aperiodic and 1-bounded.

For all $S \in Q'$, let us define $\Delta^*(S, s) = \{(q', P') \mid \exists (q, P) \in S \text{ such that } (q, P) \rightsquigarrow_{T, A}^s (q', P')\} \cap \text{useful}(T, A)$.

Claim Let $M_{T'}$ be the transition monoid of T' and $M_{T, A}$ the transition monoid of (T, A) . Let $S_1, S_2 \in Q'$, $X_{q, P}, Y_{q', P'} \in \mathcal{X}'$ and $s \in \Sigma^*$. Then one has $M_{T', s}[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = i \geq 0$ iff $S_2 = \Delta^*(S_1, s)$ and one of the following hold:

1. either $i = 0$ and, $(q, P) \notin S_1$ or $(q', P') \notin S_2$, or
2. $(q, P) \in S_1$, $(q', P') \in S_2$, (q, P) is the minimal ancestor in S_1 of (q', P') (i.e. $(q, P) = \min \{(r, R) \in S_1 \mid (q', P') \in \Delta^*((r, R), s)\}$), and $M_{(T, A), s}[(q, P), X][(q', P'), Y] = i$.

Proof of Claim. It is easily shown that $M_{T', s}[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] \geq 0$ iff $S_2 = \Delta^*(S_1, s)$. Let us show the two other conditions. Assume that $M_{T', s}[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = i \geq 0$. The variable update function is defined in such a way that after reading s from S_1 , all the variables $Z_{(r, R)}$ such that $(r, R) \notin S_2$ have just been reset to ϵ (and therefore no variable can flow from S_1 to them). In particular, if $(q', P') \notin S_2$, then no variable can flow in $Y_{(q', P')}$ and $i = 0$.

Now, assume that $(q', P') \in S_2$, and consider the sequence of states $S_1, S'_1, S'_2, \dots, S'_k, S_2$ of T' on reading s . By definition of the variable update, the variables that are used to update $Y_{(q', P')}$ on reading the last symbol of s from S'_k are copies of the form $Z_{(r, R)}$ such that (r, R) is the minimal predecessor in S'_k of (q', P') (by Δ). By induction, it is easily shown that if some variable $Z_{(r, R)}$ flows to $Y_{(q', P')}$ from S_1 to S_2 on reading s , then (r, R) is necessarily the minimal ancestor (by Δ^*) of (q', P') on reading s . In particular if $(q, P) \notin S_1$, then $i = 0$.

Finally, if $i > 0$, then necessarily (q, P) is the minimal ancestor in S_1 of (q', P') on reading s , from S_1 to S_2 , and since T' mimics the variable update of (T, A) on the copies, we get that $M_{(T, A), s}[(q, P), X][(q', P'), Y] = i$.

The converse is shown similarly.

End of Proof of Claim.

1-boundedness and aperiodicity of T' 1-boundedness is an obvious consequence of the claim and the fact that (T, A) is 1-bounded. Let us show that $M_{T'}$ is aperiodic. We know that $M_{T, A}$ is aperiodic. Therefore there exists $n \in \mathbb{N}$ such that for all strings $s \in \Sigma^*$, $M_{(T, A), s}^n = M_{(T, A), s}^{n+1}$.

Let us first show that for all $S_1, S_2 \in Q'$, and all strings $s \in \Sigma^*$, $\Delta^*(S_1, s^n) = S_2$ iff $\Delta^*(S_1, s^{n+1}) = S_2$. Indeed,

- $S_2 = \Delta^*(S_1, s^n)$, iff $S_2 = \{(q', P') \in \text{useful}(T, A) \mid \exists (q, P) \in S_1, (q, P) \rightsquigarrow_{T, A}^{s^n} (q', P')\}$, iff
- $S_2 = \{(q', P') \in \text{useful}(T, A) \mid \exists (q, P) \in S_1, M_{(T, A), s}^n[(q, P), X][(q', P'), Y] \geq 0 \text{ for some } X, Y \in \mathcal{X}\}$, iff
- by aperiodicity of $M_{T, A}$, $S_2 = \{(q', P') \in \text{useful}(T, A) \mid \exists (q, P) \in S_1, M_{(T, A), s}^{n+1}[(q, P), X][(q', P'), Y] \geq 0 \text{ for some } X, Y \in \mathcal{X}\}$, iff
- $S_2 = \Delta^*(S_1, s^{n+1})$.

Let $S_1, S_2 \in Q'$ and $X_{(q, P)}, Y_{(q', P')} \in \mathcal{X}$. Let also $s \in \Sigma^*$. We study condition (1) of the claim and show that

$M_{T', s}^n[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = i$ and condition (1) of the claim holds, iff $M_{T', s}^{n+1}[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = i$ and condition (1) of the claim holds.

- Indeed, $M_{T', s}^n[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = 0$ and, $(q, P) \notin S_1$ or $(q', P') \notin S_2$ iff (by the claim) $\Delta^*(S_1, s^n) = S_2$, and $(q, P) \notin S_1$ or $(q', P') \notin S_2$, iff by what we just showed, $\Delta^*(S_1, s^{n+1}) = S_2$, and $(q, P) \notin S_1$ or $(q', P') \notin S_2$, iff (by the claim) $M_{T', s}^{n+1}[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = 0$ and condition (1) of the claim holds.

Let us now treat condition (2) of the claim, and show that

$M_{T', s}^n[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = i$ and condition (2) of the claim holds, iff $M_{T', s}^{n+1}[S_1, X_{(q, P)}][S_2, Y_{(q', P')}] = i$ and condition (2) of the claim holds.

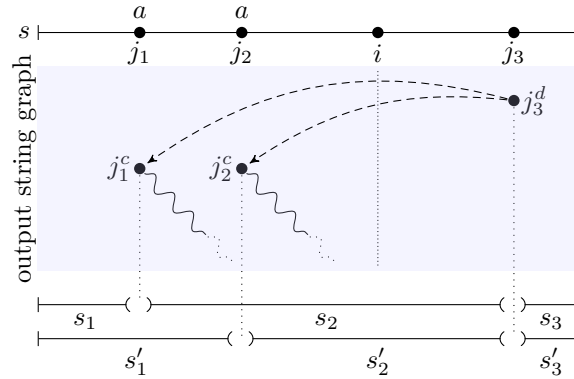
- We only show one direction, the other being proved exactly similarly. Suppose that $M_{T',s}^n[S_1, X_{(q,P)}][S_2, Y_{(q',P')}] = i$ and $(q, P) \in S_1$, $(q', P') \in S_2$, and (q, P) is the minimal ancestor in S_1 of (q', P') , and $M_{(T,A),s}^n[(q, P), X][(q', P'), Y] = i$. It implies, by the claim, that $\Delta^*(S_1, s^n) = S_2$, and therefore $\Delta^*(S_1, s^{n+1}) = S_2$. Now, we have $(q, P) = \min \{(r, R) \in S_1 \mid (q', P') \in \Delta^*((r, R), s^n)\}$. Since $\Delta^*((r, R), s^n) = \Delta^*((r, R), s^{n+1})$ for all $(r, R) \in S_1$, we have $(q, P) = \min \{(r, R) \in S_1 \mid (q', P') \in \Delta^*((r, R), s^{n+1})\}$. Finally, $M_{T,A,s}^{n+1}[q, P, X][q', P', Y] = M_{T,A,s}^n[q, P, X][q', P', Y] = i$ (by aperiodicity of (T, A)). By the claim, it implies that $M_{T',s}^{n+1}[S_1, X_{(q,P)}][S_2, Y_{(q',P')}] = i$ and condition (2) of the claim is satisfied.

Since by the claim we can be only in case (1) or (2), it implies that $M_{T'}$ is aperiodic. ◀

F Proofs from Section 5.2

F.1 Proof of Lemma 22

Proof. Intuitively, if $j_1 \neq j_2$ and j_1^c, j_2^c are both i -heads, then the string s can be decomposed as in the following figure:



Since the output is a string, there is necessarily some edge from a position j_3^d such that $j_3 > i$, to j_1^c or j_2^c . It can be easily shown that the existence of such an edge is FO-definable by a formula with two-free variables of quantifier rank at most k . Since the two decompositions are indistinguishable by formulas with two-free variables of quantifier rank at most k , by Proposition 1.2, one gets that an edge from j_3^c to the other considered i -head also exist, which contradicts the fact that the output is a string.

We formally prove the result now. Suppose that there exist $j_1 \neq j_2$ that both satisfy the preconditions and suppose that j_1^c and j_2^c are both i -heads. We exhibit a contradiction.

By definition of i -heads, j_1^c and j_2^c are alive, and therefore both contribute to the output $T(s)$. Since $T(s)$ is a string (i.e. a unique directed path), there is necessarily some incoming edge to j_1^c or j_2^c in $T(s)$, say j_1^c . Formally, there exists a position j_3 and a copy $d \in C$ such that (j_3^d, j_1^c) is an edge of $T(s)$, i.e. $s \models \phi_{\text{succ}}^{d,c}(j_3, j_1)$. Since j_1^c is an i -head, it is necessarily the case that $j_3 > i$. We claim that $s \models \phi_{\text{succ}}^{d,c}(j_3, j_2)$, i.e. there exists an edge in $T(s)$ from j_3^d to j_2^c , which contradicts the fact that $T(s)$ is a string.

Indeed, let decompose the input string s as

$$\begin{array}{ll} s_1 &= s[1:j_1] & s'_1 &= s[1:j_2] \\ s_2 &= s(j_1:j_3) & s'_2 &= s(j_2:j_3) \\ s_3 &= s(j_3:s[]) & s'_3 &= s(j_3:s[]) \end{array}$$

We show that the conditions of Proposition 1.2 are satisfied by this decomposition. Clearly, $s = s_1 s[j_1] s_2 s[j_3] s_3 = s'_1 s[j_2] s'_2 s[j_3] s'_3$. Moreover, $s_1 \equiv_{k+2} s'_1$ by hypothesis, and, $s_3 \equiv_{k+2} s'_3$ since $s_3 = s'_3$. We also have $s_2 = s(j_1:i) s(i:j_3)$ and $s'_2 = s(j_2:i) s(i:j_3)$ and by hypothesis, $s(j_1:i) \equiv_{k+2} s(j_2:i)$. Hence, by Proposition 1.1 one gets $s \equiv_{k+2} s'$. Since

$s \models \phi_{\text{succ}}^{d,c}(j_3, j_1)$, and $s \equiv_{k+2} s'$, using Proposition 1.2 we get $s \models \phi_{\text{succ}}^{d,c}(j_3, j_1)$ iff $s \models \phi_{\text{succ}}^{d,c}(j_3, j_2)$ (Recall that by definition of quantifier rank k of T , $\phi_{\text{succ}}^{d,c}$ has quantifier rank at most k). Since $s \models \phi_{\text{succ}}^{d,c}(j_3, j_1)$, one gets $s \models \phi_{\text{succ}}^{d,c}(j_2, j_1)$, which leads to the contradiction mentioned earlier. The proof is the same when assuming that j_1^c and j_2^c are both i -tails. \blacktriangleleft

F.2 Proof of Lemma 24

Proof. Let $\alpha \in \mathcal{A}_T$ and $c \in C$. Let us first prove the Lemma for the heads. Let x, y be two variables (intended to capture positions i and j respectively).

The condition that $\tau_1(\alpha) = \langle s[1:j] \rangle_{k+2}$ can be expressed, thanks to Proposition 2, by the formula $\phi_2(x, y)$ of quantifier rank at most $k+2$ obtained by guarding all the quantifications of any variable z in $\phi_{\tau_1(\alpha)}$ by $z \prec y$.

The condition $a(\alpha) = s[j]$ is expressed by the formula $\phi_3(y) = L_{a(\alpha)}(y)$.

The condition $\tau_2(\alpha) = \langle s(j:i) \rangle_{k+2}$ is defined, again by using Proposition 2, by the formula $\phi_4(x, y)$ of quantifier rank at most $k+2$, obtained by guarding all the quantifications of any variable z in $\phi_{\tau_2(\alpha)}$ by $y \prec z \preceq x$.

Finally, the formula $\Phi_{\text{HD}(\alpha)}^c(x, y)$ is defined by

$$\Phi_{\text{HD}(\alpha)}^c(x, y) \equiv \text{head}_c(x, y) \wedge \phi_2(x, y) \wedge \phi_3(y) \wedge \phi_4(x, y)$$

The formula $\text{head}_c(x, y)$ has quantifier rank at most $k+2$, therefore $\Phi_{\text{HD}(\alpha)}^c(x, y)$ has quantifier rank at most $k+2$.

The formula $\Phi_{\text{TL}(\alpha)}^c(x, y)$ is defined by

$$\Phi_{\text{TL}(\alpha)}^c(x, y) \equiv \exists z. \bigvee_{c' \in C} \Phi_{\text{HD}(\alpha)}^{c'}(x, z) \wedge \phi_{\preceq}^{c',c}(z, y) \wedge \forall z' > x. \neg \bigvee_{c'' \in C} (\phi_{\preceq}^{c',c''}(z, z') \wedge \phi_{\preceq}^{c'',c'}(z', y))$$

This formula has quantifier rank at most $k+3$. \blacktriangleleft

G Proofs from Section 5.3

G.1 T_{la} admits exactly one accepting runs per string $s \in \text{dom}(T_{\text{la}})$

Proof. For any two transitions $(\tau_1, a, p_\tau, \tau_1'), (\tau_2, a, p_{\tau'}, \tau_2')$ of T_{la} , if $\tau_1 = \tau_2$, then on suffix $u \in \Sigma^*$, at most one of the two transitions can be triggered, because u cannot satisfy both types τ and τ' , since k -types partition Σ^* . \blacktriangleleft

G.2 Proof of Lemma 25

Proof. First, recall that the look-ahead automaton has transitions of the form $(\tau, \tau') \xrightarrow{a} (\tau, \tau'.\langle a \rangle_{k+2})$ and accepting state of the form (τ, τ) for all $(k+2)$ -types τ .

Since we assume that $s \in \text{dom}(T_{\text{la}})$, given an integer $j \in \{0, \dots, n\}$, we can precisely define the j -th configuration (q_j, P_j) of the unique accepting run r of T_{la} on s . By definition of T_{la} and its look-ahead automaton, we indeed have:

1. $q_j = \langle s[1:j] \rangle_{k+2}$ (recall that q_j is a $k+2$ -type)
2. $R_j = \{(\langle s[\ell+1:n] \rangle_{k+2}, \langle s[\ell+1:j] \rangle_{k+2}) \mid 1 \leq \ell \leq j\}$

Notice that q_0 is indeed equal to $\langle \epsilon \rangle_{k+2} = \langle s[1:0] \rangle_{k+2}$ and $R_0 = \emptyset = \{(\langle s[\ell+1:n] \rangle_{k+2}, \langle s[\ell+1:j] \rangle_{k+2}) \mid 1 \leq \ell \leq 0\}$. Let us express equalities 1. and 2. in FO.

We construct a formula $\Phi_{q,R}(x)$ such that $s \models \Phi_{q,R}(j)$ iff $(q, R) = (q_j, R_j)$, for all positions $j \in \text{dom}(s)$. It is defined by:

$$\Phi_{q,R}(x) \equiv \Phi_q^{\preceq x}(x) \wedge \Phi_R(x)$$

where $\Phi_q^{\preceq x}(x)$ expresses the fact that the prefix up to position x has type q , and is obtained by guarding all the quantifiers of Φ_q (the Hintikka formula corresponding to type q , see Proposition 2) by $\preceq x$. The formula $\Phi_R(x)$ expresses the fact that the look-ahead states after reading position x are R :

The second property is expressed by the conjunction of the two following formulas $\Phi_R^2(x)$ and $\Phi_R^3(x)$, where

$$\Phi_R^2(x) = \forall z \cdot (1 \preceq z \preceq x \rightarrow \bigvee_{(\tau, \tau') \in R} \Phi_\tau^{z \prec \cdot} \wedge \Phi_{\tau'}^{z \prec \cdot \preceq x})$$

$$\Phi_R^3(x) = \bigwedge_{(\tau, \tau') \in R} \exists z \cdot 1 \preceq z \preceq x \wedge \Phi_\tau^{z \prec \cdot} \wedge \Phi_{\tau'}^{z \prec \cdot \preceq x}$$

where the superscript $z \prec \cdot$ and $z \prec \cdot \preceq x$ indicates the guards applied to the quantifiers.

Finally, the formula $\text{sflow}_{q,q',R,R'}(x,y)$ is defined by distinguishing among the cases $x = y = 1$, $x = 1 \prec y$ and $1 \prec x \preceq y$:

$$\begin{aligned} \text{sflow}_{q,q',R,R'}(x,y) &\equiv x \preceq y \wedge \\ &(x = y = 1 \wedge \Psi_{q=q_0, R=\emptyset} \wedge \Psi_{q'=q_0, R'=\emptyset}) \vee (x = 1 \prec y \wedge \Psi_{q=q_0, R=\emptyset} \wedge \Phi_{q',R'}(y)) \vee (x > 1 \wedge \Phi_{q,R}(x-1) \wedge \Phi_{q',R'}(y)) \end{aligned}$$

where $\Psi_{q=q_0, R=\emptyset} \equiv \top$ if $q = q_0$ and $R = \emptyset$, otherwise \perp , and similarly for $\Psi_{q'=q_0, R'=\emptyset}$. The formula $\text{sflow}_{q,q',R,R'}(x,y)$ has a quantifier rank at most $k+3$. \blacktriangleleft

G.3 Proof of Lemma 27

Proof. We define two different formulas, depending on whether $m = 0$ or $m \geq 1$.

Suppose first that $m \geq 1$. We show how to define the formula $\text{rflow}_t(x,y)$ in FO by expressing the conditions of Lemma 26 and taking the resulting formula in conjunction with the formula $\text{sflow}_{q,q',R,R'}(x,y)$ obtained from Lemma 25. One uses two free variables x' and y' to extract the x - and y -heads corresponding to adresses α and α' , thanks to Lemma 24. The whole formula is defined by:

$$\begin{aligned} \text{rflow}_t(x,y) &\equiv \text{sflow}_{q,q',R,R'}(x,y) \wedge \bigvee_{c,c' \in C} \exists x' \exists y' \Phi_{\text{HD}(\alpha)}^c(x,x') \wedge \Phi_{\text{HD}(\alpha')}^{c'}(y,y') \wedge \Phi_{\preceq}^{c',c}(y',x') \wedge \\ &\neg \exists z [z > y' \wedge \bigvee_{c'' \in C} \Phi_{\preceq}^{c',c''}(y',z) \wedge \Phi_{\preceq}^{c'',c}(z,x')] \end{aligned}$$

This formula has quantifier rank at most $k+4$.

If $m = 0$, then the formula $\text{rflow}_t(x,y)$ is obtained by taking the conjunction of the negation of the previous formula with the formula $\text{sflow}_{q,q',R,R'}(x,y)$. \blacktriangleleft

G.4 Proof of Lemma 28

Proof. We have to distinguish two cases, depending on whether $|s| = 0$ or $|s| > 0$. For these two cases, we construct two formula flow_t^0 and $\text{flow}_t^{>0}$, and then define flow_t by

$$\text{flow}_t \equiv \text{flow}_t^0 \wedge \text{flow}_t^{>0}$$

In case $|s| = 0$, it should be true that $q = q'$, $R = R'$, $X_\alpha = X_{\alpha'}$ and $m = 1$. It is defined by the formula

$$\text{flow}_t^0 \equiv (\neg \exists x. \top) \rightarrow B_{q=q', R=R', \alpha=\alpha', m=1}$$

where $B_{q=q', R=R', \alpha=\alpha', m=1} = \top$ if indeed $q = q'$, $R = R'$, $\alpha = \alpha'$ and $m = 1$, and \perp otherwise.

Then, we consider the case $|s| > 0$ and construct the formula $\text{flow}_t^{>0}$ as follows. We first transform the formula $\text{rflow}_t(x,y)$ into a sentence rflow_t^{xy} on the FO-signature whose alphabet is extended with pairs of Boolean values that indicate the positions of x and y respectively, so that $s \models \text{rflow}_t(i,j)$ iff $(s,i,j) \models \text{rflow}_t^{xy}$, where (s,i,j) is the string s extended with the pair $(0,1)$ at position i , the pair $(1,0)$ at position j , and the pairs $(0,0)$ elsewhere.

The formula rflow_t^{xy} is defined by $\exists x \exists y [\text{rflow}_t'(x,y) \wedge \bigvee_{a,b \in \Sigma} L_{(a,0,1)}(x) \wedge L_{(b,1,0)}(y)]$ where $\text{rflow}_t'(x,y)$ is obtained by replacing all atoms of the form $L_a(z)$ by $\bigvee_{b_1, b_2 \in \{0,1\}} L_{a,b_1,b_2}(z)$ in $\text{rflow}_t(x,y)$.

Since rflow_t^{xy} is an FO-formula, there exists an aperiodic automaton over the alphabet $\Sigma \times \{0, 1\}^2$ that defines the same language. We intersect this automaton with an (aperiodic) automaton that checks that the sequence of Boolean pairs belongs to $(0, 0)^*(0, 1)(0, 0)^*(1, 0)(0, 0)^*$. Let L^b (b for Boolean) denote the aperiodic language defined by this automaton.

Let us define the language L of strings u over $\Sigma \times \{0, 1\}^2$ whose sequence of Boolean pairs is in $(0, 1)(0, 0)^*(1, 0)$ and such there exists $u_1, u_2 \in (\Sigma \times \{(0, 0)\})^*$ such that $u_1 u u_2 \in L^b$. The language L can be easily defined by some aperiodic automaton obtained from any aperiodic automaton defining L^b . We now define the language $\pi(L)$ obtained by projecting L on the component Σ , i.e. $\pi(L)$ is the set of strings s such that s can be extended with Boolean pairs into a string u such that $u \in L$. The language $\pi(L)$ is aperiodic. Indeed, there is a bijection between the strings s of $\pi(L)$ to the strings L , defined by extending the first symbol of s with $(0, 1)$, its last symbol by $(1, 0)$, and the symbols in between by $(0, 0)$. Aperiodic languages are not closed by projection in general, but they are preserved by bijective renaming [12]. Therefore $\pi(L)$ is aperiodic, and definable by some FO formula $\Phi_{\pi(L)}$. We let $\text{flow}_t^{>0} = (\exists z. \top) \rightarrow \Phi_{\pi(L)}$.

Let us prove the correctness of $\text{flow}_t^{>0}$. Suppose that $s \models \text{flow}_t^{>0}$ and $|s| > 0$. Therefore there exists an extension u of s on the alphabet $\Sigma \times \{0, 1\}^2$ such that $u \in L$, i.e. $u \in L$. By definition of L , the Boolean part of u is necessarily of the form $(0, 1)(0, 0)^*(1, 0)$, and there exist $u_1, u_2 \in (\Sigma \times \{(0, 0)\})^*$ such that $u_1 u u_2 \models L^b$. By definition of L^b , we get $u \models \text{rflow}_t^{xy}$, i.e. $s_1 s s_2 \models \text{rflow}_t(i, j)$, where s_1, s_2 are the projections of u_1, u_2 on Σ , i is the starting position of s and j its ending position. In other words, $(q, R, X_\alpha) \rightsquigarrow_m^{(s_1 s s_2)[i:j]} (q', R', X_{\alpha'})$ and in particular, $(q, R, X_\alpha) \rightsquigarrow_m^s (q', R', X_{\alpha'})$.

Conversely, suppose that $(q, R, X_\alpha) \rightsquigarrow_m^s (q', R', X_{\alpha'})$ with $|s| > 0$. Since (q, R) and (q', R') are useful, there exists s_1, s_2 such that there exists a run from the initial pair (q_0, R_0) to (q, R) on s_1 , and there exists an accepting run from (q', R') to an accepting pair on s_2 . In particular $s_1 s s_2 \in \text{dom}(T_{\text{la}})$. Therefore $(q, R, X_\alpha) \rightsquigarrow_m^{(s_1 s s_2)[i:j]} (q', R', X_{\alpha'})$, where i and j are respectively the starting and ending position of s in $s_1 s s_2$. Therefore $s_1 s s_2 \models \text{rflow}_t(i, j)$. If one extends s_1 with Boolean pairs $(0, 0)$, s with $(0, 1)(0, 0)^{n-2}(1, 0)$, where $n = |s|$, and s_2 with the Boolean pairs $(0, 0)$, one gets three strings u_1, u, u_2 such that $u_1 u u_2 \models \text{rflow}_t^{xy}$, i.e. $u_1 u u_2 \in L^b$. By definition of L , we also get $u \in L$ and thus $u \in L$ and clearly, s (the projection of u on Σ) satisfies $\text{flow}_t^{>0}$. ◀

G.5 Proof of Corollary 29

Proof. From Lemma 28, it is clear that T_{la} is 1-bounded. We show that the transition monoid M of T_{la} is aperiodic. Let $s \in \Sigma^*$ and let $t = (q, q', R, R', X_\alpha, X'_\alpha, m) \in Q \times Q \times 2^{Q_A} \times 2^{Q_A} \times X \times X \times \mathbb{N}$.

If (q, R) is not useful or (q', R') is not useful, then for all m , $M_{s^m}[q, R][q', R'] = \perp$.

Now suppose that (q, R) and (q', R') are both useful. By Lemma 28, there exists an FO-sentence flow_t such that $s \models \text{flow}_t$ iff $(q, R, \alpha) \rightsquigarrow_n^s (q', R', \alpha')$. Let b be the maximal quantifier rank of all the formulas flow_t . By Proposition 1.3 there exists n_0 such that $s^{n_0} \equiv_b s^{n_0+1}$. Therefore there exists n_0 such that for all tuples t , $s^{n_0} \models \text{flow}_t$ iff $s^{n_0+1} \models \text{flow}_t$, i.e. $(q, R, \alpha) \rightsquigarrow_m^{s^{n_0}} (q', R', \alpha')$ iff $(q, R, \alpha) \rightsquigarrow_m^{s^{n_0+1}} (q', R', \alpha')$. In other words $M_{s^{n_0}}[(q, R, \alpha)][(q', R', \alpha')] = m$ iff $M_{s^{n_0+1}}[(q, R, \alpha)][(q', R', \alpha')] = m$. Therefore the transition monoid of T_{la} is aperiodic. ◀

H f_{halve} is not FO-definable

Proof. Let assume that it is FO-definable by some FO-transducer T that outputs strings over a signature that does not contain the transitive closure of the successor relation. We show a contradiction, which will therefore imply the non FO-definability of f_{halve} by an FO-transducer that, additionally, must output the transitive closure of the successor relation.

Let $k = \text{qr}(T)$ be the quantifier rank of T , and $C > 0$ be the number of copies of T . We know by Proposition 1.3 that for all $n \geq 2^{k+2}$, $a^n \equiv_{k+2} a^{n+1}$. Take such an n and consider the string $s := a^{8nC}$.

Clearly, $f_{\text{halve}}(s) = a^{4nC}$. Therefore the output graph of $T(s)$ contains $4nC - 1$ edges. Suppose that $s \models \phi_{\text{succ}}^{c,d}(i, j)$ for some copies c, d of T and some input positions $i \leq j$ (the case $j \leq i$ is symmetric).

Suppose that $j - i > n$ and $i > n$. Therefore $s[1:i-1] = a^{i-1} \equiv_{k+2} a^i = s[1:i-1]$ and $s[i, j] = a^{j-i+1} \equiv_{k+2} a^{j-i} = s[i+1, j]$. Since $s \models \phi_{\text{succ}}^{c,d}(i, j)$ and the quantifier rank of $\phi_{\text{succ}}^{c,d}$ is at most k , by Proposition 1.2, it is also the case that

$s \models \phi_{\text{succ}}^{c,d}(i-1, j)$. It is a contradiction since in that case, there would be two incoming edges to the output node j^d , and the output would not be a string.

A similar contradiction being obtained symmetrically for the case $j-i > n$ and $j < 8nC - n$, it implies that necessarily, if $j-i > n$, then $i \leq n$ and $j \geq 8nC - n$. In other words, either the edge (i^c, j^d) is “local” or one of its element is close from the extremities of s . In both cases, we show again a contradiction.

Now, there exist necessarily two positions i', j' and two copies c', d' such that $s \models \phi_{\text{succ}}^{c',d'}(i', j')$ such that $n < i'$ and $j' < 8nC - n$. If it was not the case, then since the input nodes in $[1, n]$ and $[8nC - n, 8nC]$ contribute to at most $2nC$ edges (otherwise the output would not be a string as two edges would have either same target or same source), there would not be a sufficient number of edges to define the output.

Therefore, since $n < i'$ and $j' < 8nC - n$, we have just shown that necessarily, it is the case that $|i' - j'| \leq n$. Since $s \models \phi_{\text{succ}}^{c',d'}(i', j')$, by a similar reasoning as before (in particular by applying Proposition 1.2), we can show that many other edges can be obtained by shifting the edge $(i'^{c'}, j'^{d'})$ left or right. More precisely, for all $\ell \in \mathbb{Z}$ such that $\max(i' + \ell, j' + \ell) \leq 7n$ and $\min(i' + \ell, j' + \ell) \geq n$, it is the case that $s \models \Phi_{\text{succ}}^{c',d'}(i' + \ell, j' + \ell)$. Since there exist at least $8nC - 3n$ such ℓ (because $|i' - j'| \leq n$ and $n < i'$ and $j' < 8nC - n$), it means that the output graph of s by T contains at least $8nC - 3n$ edges, which is a contradiction. Indeed, we know that the output contains exactly $4nC - 1$ edges, and $8nC - 3n - 4nC + 1 = 4nC - 3n + 1 > 0$. ◀